LLNL-TR-413767

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Physical and Life Sciences 2008 Science & Technology Highlights

D. L. Correll, A. U. Hazi

June 9, 2009

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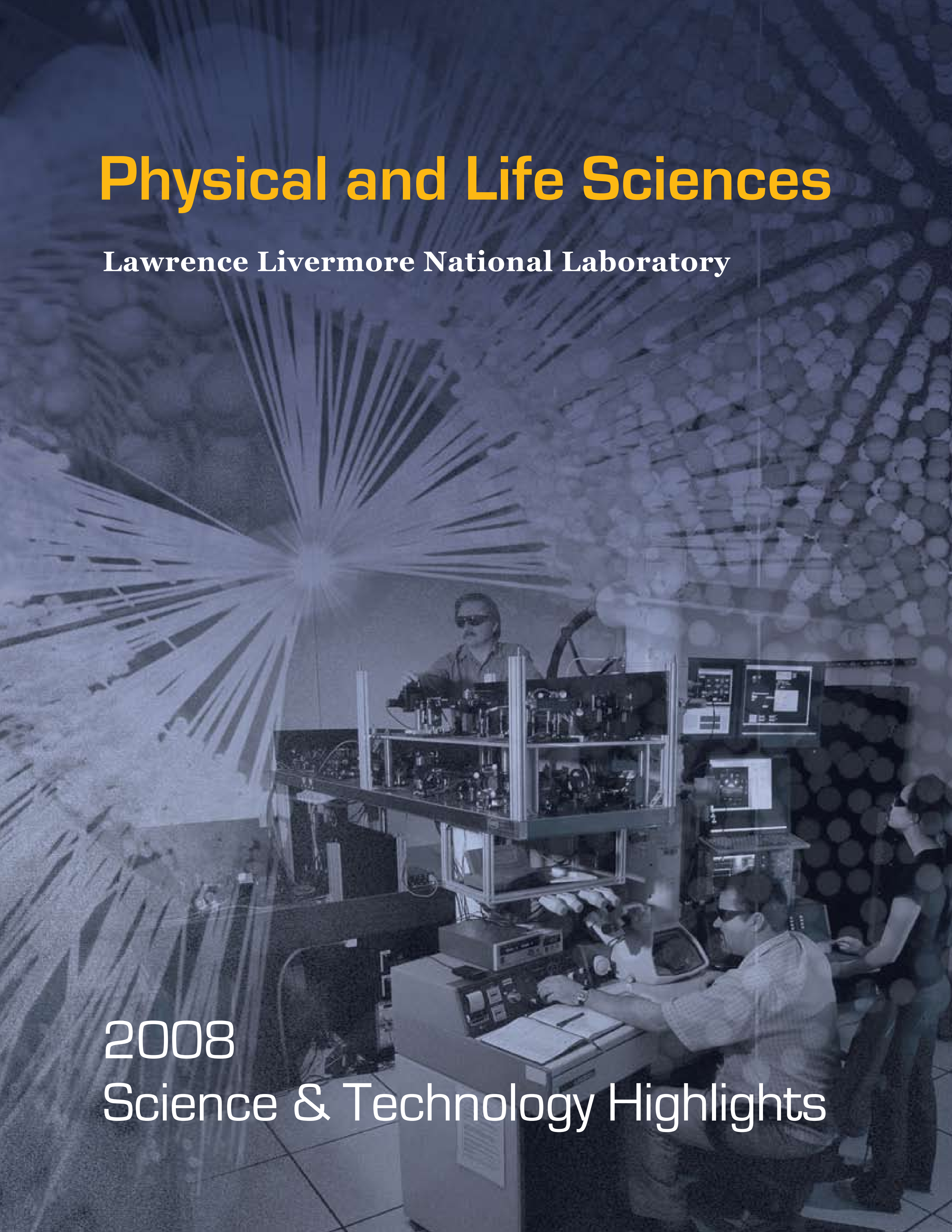
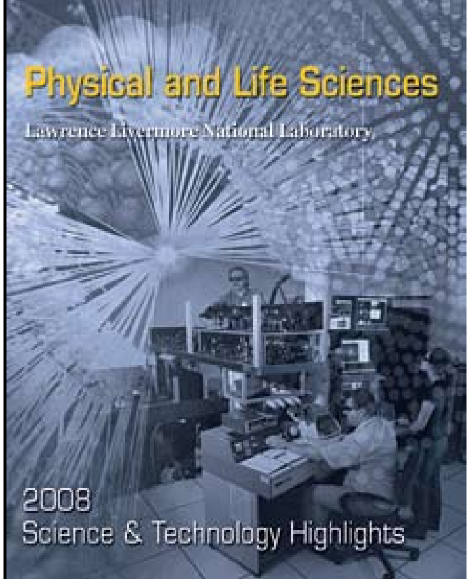
Physical and Life Sciences

Lawrence Livermore National Laboratory



2008

Science & Technology Highlights



About the Cover

A photo of researchers with the new dynamic transmission electron microscope (DTEM) they helped develop (see "New electron microscope takes nanosecond snapshots of materials," on page 23) is shown against a background of scientific images from other recent achievements in the Physical and Life Sciences (PLS) Directorate. This collage encapsulates the breadth of science disciplines in PLS—physics, chemistry, materials sciences, earth sciences, and life sciences. This broad range of science enables PLS to achieve its mission of creating and applying knowledge that advances the security and well-being of the nation.

About this Report

This document highlights the outstanding research and development activities in the Physical and Life Sciences Directorate that made news in 2008. It also summarizes the awards and recognition received by members of the Directorate in 2008.

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This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Security, LLC, Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

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Find Out More About Us

Visit our Web site at *https://www-pls.llnl.gov/* for more information on Physical and Life Sciences research, facilities, publications, staff, organization, events, and awards.

Directorate Overview

Valuing integrity, innovation, and impact

Overview

On October 1, 2008, Laboratory Director George Miller announced the integration of the Chemistry, Materials, Earth and Life Sciences Directorate and the Physical Sciences Directorate to form the Physical and Life Sciences (PLS) Directorate. With this integration, the PLS, Computation, and Engineering Directorates together constitute the Laboratory's Science and Technology Principal Directorate. William Goldstein, who was previously the Associate Director (AD) for Physical Sciences, now serves as the AD for PLS. The new PLS Directorate has a budget of over $150 million and a staff of approximately 800 employees.

This integration of two major science disciplinary organizations at the Laboratory has allowed the combination and alignment of synergistic scientific elements to create stronger disciplines and to provide more effective and cost-efficient support to LLNL programs.

Mission

The mission of PLS is to enable the Laboratory to accomplish its primary fundamental science objectives through excellence in the physical and life sciences in the areas of weapons and complex integration, National Ignition Facility and photon science, and global security. The directorate partners with other LLNL programs and disciplines to accomplish the Laboratory's mission to advance and apply science and technology to:

- Ensure the safety, security, and reliability of the U.S. nuclear deterrent.
- Reduce or counter threats to national and global security.
- Enhance the energy and environmental security of the nation.
- Strengthen the nation's economic competitiveness.

Goals

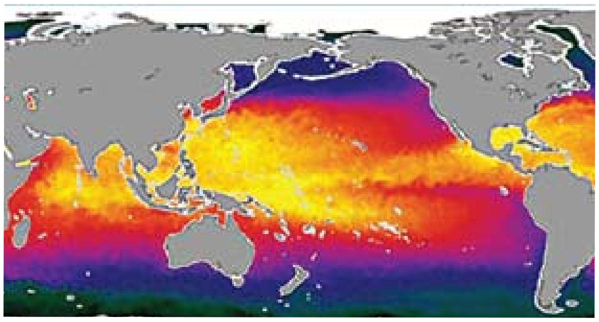
The PLS Directorate *(http://www-pls.llnl.gov)* delivers science that ensures the success of the LLNL's national security programs, anticipates their future needs, and provides innovative solutions to some of the hardest scientific problems facing the nation. To achieve these goals, the PLS Directorate:

- Attracts, trains, and retains a world-class scientific workforce for the Laboratory's national security missions.
- Maintains specialized research capabilities and facilities to provide leadership in broad research areas of the physical and life sciences that are central to LLNL's missions.
- Combines unique expertise and capabilities in measurement science, simulation, and theory to find solutions for national security problems and to advance the scientific foundations of the Laboratory.

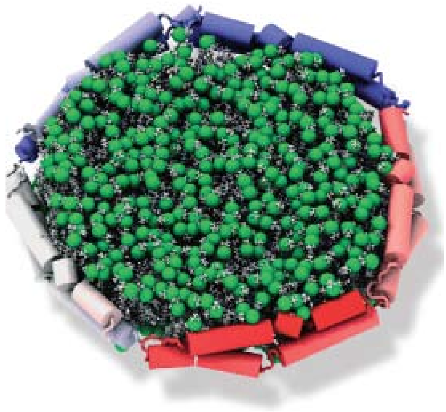
Divisions

The PLS Directorate is organized along disciplinary lines into five divisions to support the R&D activities that place LLNL at the leading edge of 21st-century national security missions:

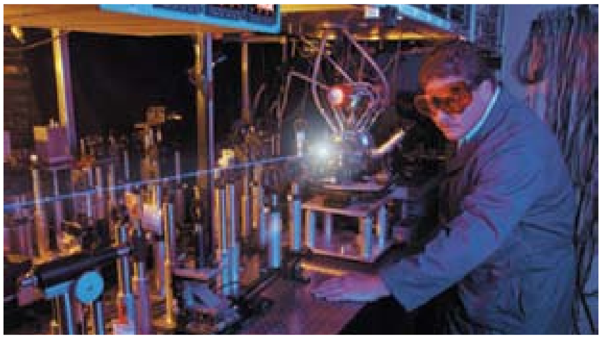
The **Atmospheric, Earth, and Energy Division** (AEED) supports the Laboratory's defense, global security, and fundamental science programs by conducting research and development in the areas of atmospheric, earth, and energy sciences. This division also supports LLNL's Center for Accelerator Mass Spectrometry, which specializes in measuring ultralow concentrations of long-lived radioisotopes. The AEED also supports programs in energy and environmental security, nonproliferation, the National Atmospheric Release Advisory Center, and the DHS Inter-Agency Modeling and Atmospheric Assessment Center.



The **Biosciences and Biotechnology Division** (BBTD) performs research in the areas of genome biology, computational biology, molecular toxicology, host–pathogen biology, biochemical structures, assays, genetics, and microbial systems. The BBTD works at the intersection of these areas using advances in nanotechnology and in imaging and measurement science.



The **Chemical Sciences Division** (CSD) conducts R&D at the intersection of chemical and nuclear science in support of LLNL's programmatic missions. Personnel in CSD provide expertise in organic and inorganic synthetic, analytical, computational, nuclear, and environmental chemistry—as well as engineering and physics—to solve problems in stockpile stewardship and other national security programs. The CSD has world-class capabilities in energetic and advanced multifunctional materials creation and characterization, nuclear chemistry and engineering, radiation detection, chemical and nuclear forensics, and environmental chemistry.



The **Condensed Matter and Materials Division** (CMMD) is the center of LLNL's integrated and comprehensive condensed-matter physics and materials science core competencies. The CMMD provides innovative and responsive science in support of the programs and performs discovery-class science ahead of the programs. Scientists in CMMD play leadership roles in the scientific community in these key and emerging areas of condensed matter and materials science.

The **Physics Division** conducts frontier physics research and development in fields ranging from astrophysics and planetary science to atomic, nuclear, and particle physics, as well as plasma and high-energy-density physics. This work includes advanced science and technology development in optical and x-ray science, detectors, accelerators, lasers, space, and fusion.

Centers and Institutes

The PLS Directorate teams with other LLNL programs to provide the additional capabilities available at its research centers and institutes. Typically multidisciplinary in nature, these organizations are staffed by personnel from our five divisions and by colleagues from across the Lab. The centers and institutes provide environments and facilities in which researchers with differing yet complementary expertise can work together on significant problems in basic and applied science and technology.

The **Center for Accelerator Mass Spectrometry** applies a wide range of isotopic and ion-beam analytical tools used in basic research and technology development to address a spectrum of scientific needs important to the Laboratory, the academic community, and the nation.

The **Center for National Security Applications of Magnetic Resonance** explores the application of nuclear magnetic resonance to national defense challenges and the characterization of biological materials.

The **Energetic Materials Center** conducts research and development on high explosives, rocket and gun propellants, and energetic materials for homeland security, demilitarization, and industrial applications.

The **Forensic Science Center** provides nationally recognized capabilities and expertise in chemical, nuclear, biological, and high-explosives forensic science to support Laboratory and national programs in counterterrorism.

The **Glenn T. Seaborg Institute** fosters collaborations between LLNL and the academic community in radiochemistry and nuclear forensics through world-class research in the areas of nuclear forensics and attribution, radiochemistry diagnostics for the National Ignition Facility, and environmental radiochemistry.

The **Institute of Geophysics and Planetary Physics**—a branch of a University of California multicampus research unit—performs basic research in the geosciences, astronomy, astrophysics and space sciences, with a current emphasis on extrasolar planet detection, large sky surveys, stellar evolution calculations, terrestrial geophysics, and astromaterials analysis.

The **Institute for Laser Science Applications** (ILSA) facilitates academic collaborations involving one or more of the Jupiter Laser Facility systems. The mission of ILSA is to strengthen the research interactions in the field of high-power lasers and their applications between LLNL and the academic community and to facilitate training and research for university students and faculty in areas important to the DOE in high-energy-density science with lasers.

The **Joint Genome Institute** (JGI) is a "virtual institute" that integrates the genomic capabilities of LLNL and five other partner institutions. The JGI provides comprehensive, high-throughput sequencing and computational analysis to enable genomic-scale and systems-based scientific approaches to national challenges in the areas of energy and the environment.

The **Jupiter Laser Facility** (JLF) is an institutional user facility that houses a variety of lasers and target chambers. The JLF provides a unique platform for the use of ultra-intense, petawatt-class lasers to explore laser–matter interactions under extreme conditions. The ILSA facilitates academic collaborations and use of the facility by faculty, postdoctoral researchers, and graduate students.

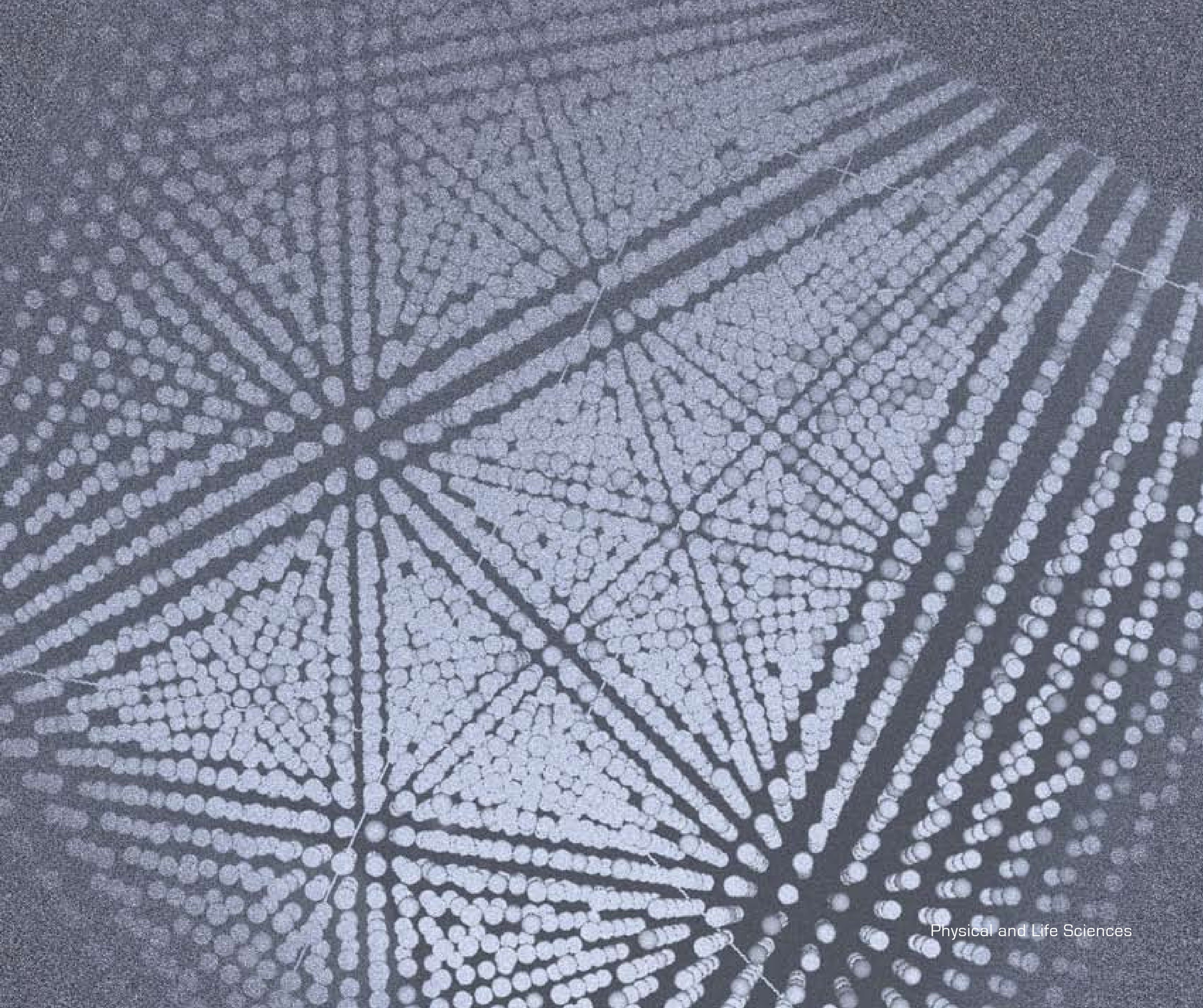
The **Livermore Microarray Center** provides microarray capabilities for numerous applications, including gene expression, comparative genomics, gene resequencing, and a wide range of forensic analyses.

The **Nanoscale Synthesis and Characterization Laboratory** conducts research on the synthesis, properties, fabrication, and performance of materials on an atomic scale. Current areas of emphasis include nanoporous materials, advanced nanocrystalline materials, three-dimensional nanofabrication technologies, and nondestructive characterization.

The **National Resource for Biomedical Accelerator Mass Spectrometry** was established to make accelerator mass spectrometry available to biomedical researchers who need to accurately measure very low levels of carbon-14. Located inside the Center for Accelerator Mass Spectrometry, this national user facility specializes in the biomedical uses of carbon-14 and tritium and also uses AMS to measure other isotopes, such as calcium-41 and beryllium-10.

Research in the News

Advancing science and technology in the national interest



Physics

Analysis of cometary dust particles reveals unexpected results

Taking advantage of Livermore's state-of-the-art electron microscopes, PLS researchers, together with collaborators in Europe, have continued their analysis of dust particles that were collected from Comet Wild 2 and then returned to Earth by NASA's Stardust spacecraft. (NASA's Stardust mission returned to Earth in January of 2006 after a 7-year mission, during which it flew by Comet Wild 2, capturing dust particles in silica aerogel tiles and aluminum foils.) In a paper published in the January 25, 2008 issue of ***Science***, Stardust researchers reported that the most abundant and most recognizable silicate materials found in interplanetary dust particles appear absent in the samples from Wild 2. In fact, the researchers were able to produce look-alikes of one of those materials in the laboratory by firing grains of minerals into Stardust collector material at the appropriate impact speeds. These results—in combination with the low abundance of bona fide presolar grains, low abundance of refractory carbon, and the presence of refractory particles normally found in meteorites—put Wild 2 in a new light. The Stardust samples show that many components in Wild 2 resemble those in meteorites from the asteroid belt in the inner solar system, indicating that the distinction between asteroids and comets is not sharp. Instead, a continuous transition exists between them, and Stardust sampled a single comet on that continuum. Now the question remains: what type of comets are the sources of the more pristine, cosmically primitive cometary interplanetary dust particles that are collected in the stratosphere by high-altitude aircraft? While only further research will be able to answer this question, the ongoing studies of the cometary material collected by Stardust are changing the understanding of the birth and childhood of our solar system.

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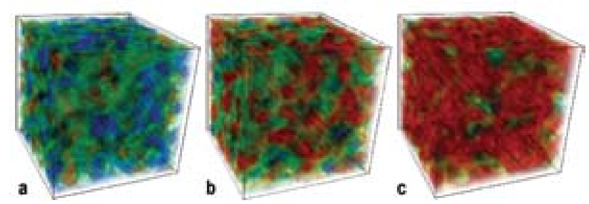
Unraveling the interactions of subatomic particles

PLS physicists are part of a large, international collaboration that used the Relativistic Heavy Ion Collider (RHIC) at Brookhaven National Laboratory to blast gold ions into individual quarks in an effort to re-create the phase transition from quarks to larger subatomic particles, such as neutrons and protons. The team succeeded in freeing the constituent quarks very briefly, but they observed some unexpected results. Instead of a hot, energized gas in which particles did not interact—a plasma—they found strong particle interactions; current models are only partially successful in explaining the observations. PLS scientists, working with theoretical physicists from around the world, are using Livermore's BlueGene/L, one of the world's fastest computers at Livermore, to understand better the quark–gluon phase transition.



A lattice quantum chromodynamics simulation shows that when matter is heated to about 170 megaelectronvolts, or about 2 trillion degrees, it melts into a quark–gluon plasma. (a) Protons, neutrons, and other nuclear particles exist below the transition temperature. (b) When the transition occurs, (c) a hot plasma emerges full of quarks and gluons. Blue indicates confined quarks, and red indicates deconfined quarks.

The researchers are using the theory of quantum chromodynamics (QCD), based on mathematics and the basic laws of physics, to calculate the conditions surrounding the transition from quarks to larger particles that was observed at RHIC. A new collaboration with Los Alamos National Laboratory, called HotQCD, is starting work to better understand the nature of the transition; how the gold ions were heated; what happened when neutrons and protons broke apart into quarks, gluons, and millions of other particles; or how quarks and gluons moved in the final hot plasma. The team's goal is to determine the condition of the plasma when the phase transition occurred—that is, the plasma's temperature, pressure, and energy, or its equation of state. With the information from the RHIC experiments, the team aims to "reverse engineer" the conditions of the phase transition, which melted quarks and gluons into larger particles during the Big Bang.

The PLS scientists are also applying lattice QCD to better understand the interactions of subatomic particles at lower energies and temperatures as part of the Nuclear Physics with Lattice QCD collaboration, made up of nuclear physicists from around the world. This collaboration has produced the first predictions of scattering lengths for several combinations of particles, including pion–pion and pion–kaon, which appeared in the February 29, 2008 issue of ***Physical Review Letters.*** Scattering lengths are a measure of the strength of the interactions between the particles. Since these particles have a very short half-life, they are difficult to measure experimentally. In 2008, the Livermore team also completed the first fully dynamic lattice QCD calculation describing the scattering of a nucleon and a hyperon, a more exotic particle.

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Properties of fluid helium at high pressure

PLS scientists and their collaborators at France's Atomic Energy Commission in Bruyères-le-Châtel, the University of California at Berkeley, and the Laboratory for Laser Energetics in Rochester measured the equation of state of fluid helium at pressures near 100 gigapascals with sufficient accuracy to test theoretical predictions. Knowledge of the properties of dense fluid helium is critical to understanding the evolution and internal structure of Jupiter, Saturn, and extrasolar giant planets. In experiments with the Omega laser in Rochester, the researchers applied laser-driven shocks to helium samples that were precompressed statically in small diamond-anvil cells. With this technique, the researchers were able to obtain shock data for a range of initial densities between one and three times the density of cryogenic liquid helium, and to separate the effects of temperature and density on the equation of state. The results show a significant increase in compressibility of helium at the onset of ionization, corresponding to an insulator-to-metal transition in the fluid—similar to theoretical predictions. This research was published in the March 28, 2008 issue of ***Physical Review Letters.*** Plans are underway to extend the research in future experiments on the National Ignition Facility, which will significantly increase the accessible range of pressures and densities, as well as the accuracy of the shock measurements, to provide further discrimination among current theoretical approaches.

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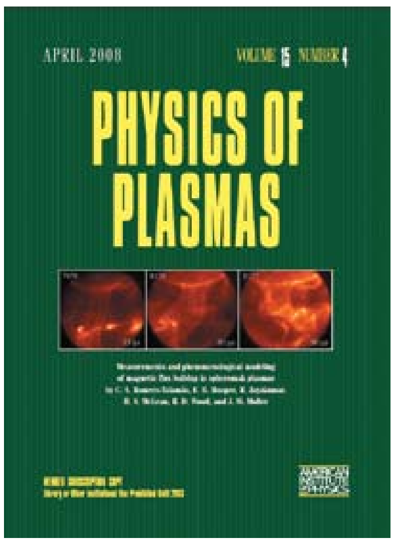
Understanding magnetic flux buildup in spheromak plasmas

A spheromak is a magnetic confinement concept for fusion plasmas, in which the stabilizing magnetic field is largely self-generated through plasma currents, leading to a stable, typically toroidal plasma. In contrast to tokamaks, spheromak devices have relatively simple designs, which require only one set of magnetic coils. A plasma gun at one end of the device ionizes the gas to form the initial plasma, which coalesces into a stable configuration. Spheromak plasmas and magnetized plasmas generated by the Sun and other celestial bodies share many of the same properties, including reconnection of the magnetic flux surfaces.

PLS researchers have made significant advances in understanding the formation and buildup of the magnetic flux in spheromak plasmas. They used internal magnetic field probes and high-speed imaging at the Sustained Spheromak Physics device at Livermore to make detailed measurements of the temporal evolution of the plasma. The scientists analyzed the measurements in terms of a phenomenological model of magnetic helicity or flux rope. During the initial phase of plasma formation, they observed large kinks in the open magnetic flux surfaces that coincide with large asymmetries detected with insertable field probes. A short time later, the flux surfaces reconnected into a closed configuration. In the second phase—buildup—the closed flux increased in discreet steps as the gun injected a train of high-current pulses into the plasma. In this phase, the researchers observed a time lag between open and closed flux surfaces after each current pulse, which they interpreted as the time for the open flux to build helicity (turns in the rope) before transferring it through reconnection to the closed flux. The large asymmetries seen during this phase relax to a slowly decaying, spheromak configuration before the next current pulse. The paper describing these results was featured on the cover of April 2008 edition of ***Physics of Plasmas.***



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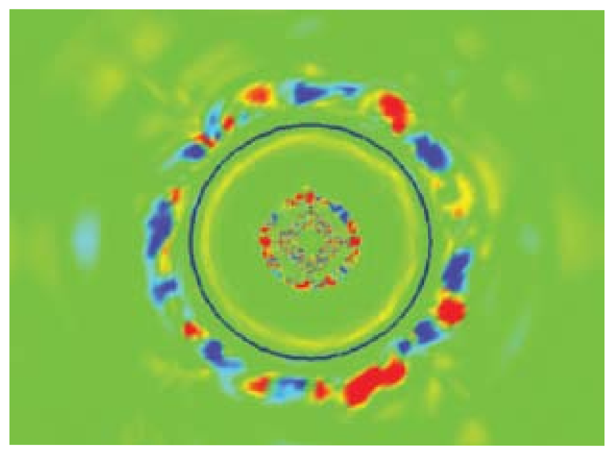
Astrophysicists solve two longstanding mysteries about the universe

Using a three-dimensional (3D) model run on some of the fastest computers in the world, Laboratory astrophysicists have cracked two mysteries of stellar evolution that have puzzled the astronomical community for years. Physicists and astronomers have long theorized that low-mass stars produce great amounts of helium-3. However, observations show that the helium-3 concentration in the interstellar medium is 100 times smaller than predicted by calculations. Using the Livermore-developed 3D code Djehuty, PLS physicists uncovered a mixing mechanism that not only accounts for the mysteriously missing helium-3, but also could explain another mystery: the overabundance of carbon-13 in the interstellar medium compared to previous calculations based on 1D models.

In simulations of the helium flash in a low-mass star, the researchers found an unexpected shell of matter deep inside the star, just outside the hydrogen-burning layer but below the convection zone at the star's surface. The shell is evidence of a molecular-weight inversion—a thin layer of helium-3 surrounding a lighter weight hydrogen layer. This inversion sets up a classic Rayleigh–Taylor hydrodynamic instability, which results in a rapid mixing process. The deep mixing of the helium-3 burning region and the convection zone effectively destroys helium-3 in the surface layer, explaining why so little of this isotope appears in the material ejected during a helium flash.



A three-dimensional model of a helium flash is shown in this two-dimensional cross section. The solid, dark-blue ring is the hydrogen-burning shell. Turbulent motion occurs in the helium-burning core near the center, as expected. The unexpected ring of turbulence just outside the hydrogen shell is the result of helium-3 burning.

The deep mixing that occurs inside low-mass stars as they evolve into red giants could also explain why the concentration of carbon-13 observed in these stars is 5 to 10 times higher than predicted by earlier 1D models. When large reservoirs of burnt helium-3 bubble upward and mix with the convective envelope, carbon-12 in the envelope is mixed downward into the hot, helium-3-burning layer. In this layer, the carbon-12 can be burned to carbon- 13 and subsequently mixed back into the surface zone. The deep mixing uncovered in the Djehuty simulations thus not only accounts for the "missing" helium-3 but also could account for the overabundance of carbon-13. These results, which appeared in the April 10, 2008 issue of the ***Astrophysical Journal,*** clearly demonstrate the virtue of modeling stars in 3D, where the hydrodynamic motion evolves naturally and to a magnitude that was unexpected.

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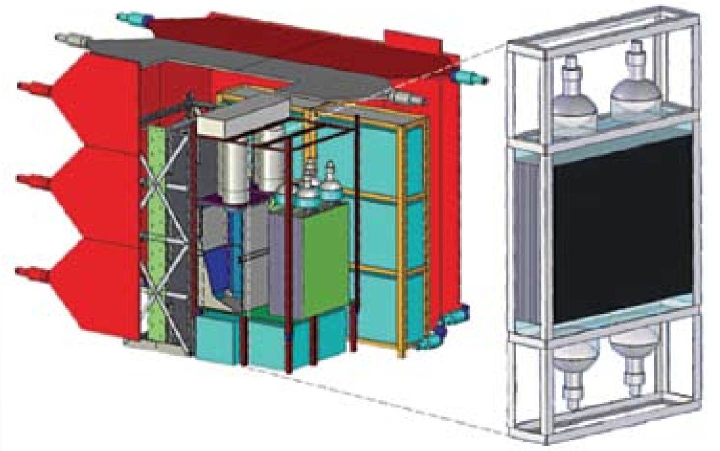
Antineutrino detectors help fight nuclear proliferation

In August 2008, three prototype antineutrino detectors developed by Lawrence Livermore and Sandia National Laboratories (SNL) were removed from the San Onofre Nuclear Generating Station (SONGS) in San Clemente, California. The first detector, called SONGS1, had been operating there since 2004; SONGS2 and SONGS3 were installed in December 2007. The autonomous detectors were developed to help the International Atomic Energy Agency (IAEA) safeguard fissile materials in nuclear reactors by providing a more precise method to confirm that reactors are operating according to IAEA standards and that fissile materials are not being diverted to a clandestine nuclear weapons program.

The detectors are designed to monitor the fission of uranium-238 and plutonium-239 inside the reactor by measuring the antineutrinos outside the reactor. The fission of both uranium and plutonium generates antineutrinos, although in substantially different amounts. The antineutrinos interact very weakly with ordinary matter, so they pass through the reactor wall undisturbed. The antineutrinos are detected through inverse beta-decay interactions. When an antineutrino collides with a proton, it produces a positron and a neutron. The interactions of these two particles create two relatively intense flashes of light, making it easy to differentiate the antineutrino signature from those resulting from other processes, such as gamma-ray or ambient neutron interactions. SONGS1 uses a proton-rich liquid scintillator doped with gadolinium to induce the inverse beta-decay interactions. SONGS2 uses alternating sheets of a plastic scintillator (instead of a liquid) and gadolinium-coated sheets. SONGS3 uses water mixed with gadolinium and measures the flashes of Cerenkov light generated in the water by the positrons and by the gamma rays resulting from the capture of neutrons by the gadolinium nuclei.



For the SONGS2 design, researchers replaced half of the liquid scintillator with a plastic scintillator (see inset). Results from field tests for the three prototypes are being analyzed to determine the effectiveness of each design.

The PLS-led team is continuing to analyze the data collected by the prototype detectors at SONGS and will test newer models at a surface location to determine the potential for aboveground operation. Using the measured antineutrino rates, the researchers have been able to estimate how quickly and how precisely a reactor's operational status and thermal power can be monitored over hour to month time scales. Analysis of the data obtained from a detector, which operated at a 25-meter standoff from a reactor core, suggests that this prototype can detect a prompt reactor shutdown within 5 hours and monitor relative thermal power to within 7 days. These results were published in the April 2008 edition of the ***Journal of Applied Physics***. The team is also working with scientists from the University of Chicago to develop argon- and germanium-based systems that will detect antineutrinos through a process called coherent neutrino–nucleus scattering. The coherent scatter process has a much higher antineutrino interaction rate per volume of detection medium compared with detectors that rely on inverse beta decay. In April 2008, the team installed the first germanium-based prototype detector at SONGS.

The research on antineutrino detection for nonproliferation applications has garnered national and international attention. The ***American Institute of Physics*** highlighted the potential of the technology in the February 5, 2008 online edition of ***Physics News Update***. ***The Institute of Physics***, in the U.K., followed with a feature in the **Headline News section of PhysicsWorld.com** on February 15, 2008. In addition, the U.S. National Academy of Engineering referenced the antineutrino detection work as one of fourteen Grand Challenges for Engineering under the category of preventing nuclear terror.

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International collaboration provides new insight into supernovae

PLS astrophysicists were members of an international collaboration that successfully identified the type of an ancient supernova in the Large Magellanic Cloud (LMC) using spectra of the light echoes surrounding the supernova remnant. Previously, the collaboration discovered light echoes associated with three ancient supernovae in the LMC using images collected by the SuperMACHO project, a 5-year microlensing survey of the LMC. The positions and motions of these echo systems indicated that the supernovae events occurred 400 to 800 years ago. The team conducted follow-up observation of the spectra of the light echoes using the multi-object spectrograph at the Gemini South observatory. By comparing and correlating the observed spectrum of one of the light echoes to spectra created from a spectral library of nearby supernovae of all types, the team found that the supernova responsible for the light echo was an especially bright, Type 1a supernova. This is the first time that the subtype of a supernova has been conclusively and directly determined long after the event had happened. These results show that light echoes provide an excellent opportunity to connect the physics of ancient supernovae to their remnants visible today. Models of supernova explosions can now be tested for consistency with the explosion itself and the observations of the supernova remnant, which will enhance the understanding of these events that play such an important role in the production of heavy elements in the universe. This research appeared in the June 20, 2008 issue of the ***Astrophysical Journal***.

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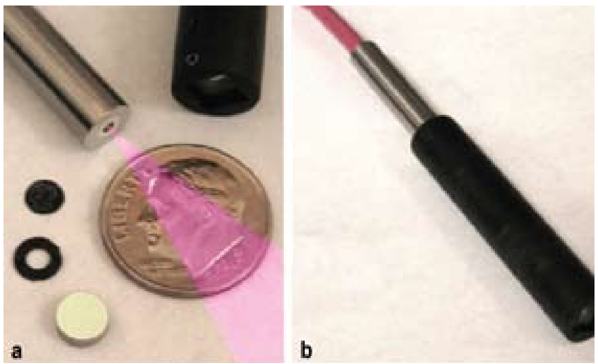
Developing new technology to monitor nuclear weapons from the inside

The NNSA is working to transform the nation's nuclear weapons complex and stockpile by shrinking their size and finding more cost-effective ways to maintain the remaining weapons. Livermore scientists and engineers are providing technical leadership to achieve this transformation. One of the most needed improvements is a cost-effective method to collect data about the state of nuclear weapon components, in particular, to detect corrosion, cracks, and composition-changing processes without having to dismantle the weapons. With funding from Livermore's Laboratory Directed Research and Development Program, a promising initiative is underway to develop tiny, rugged sensors that could be embedded in every nuclear weapon. Embedded sensors, compatible with warhead materials, could provide information currently obtained from disassembly. Once in place, an array of different sensors could signal the presence of unwanted gases, record stresses incurred as a warhead is moved, and detect microscopic cracks and voids. Being able to assess every weapon in real time would make it possible to immediately know which warheads need to be disassembled, which would reduce costs.



(a) The components used for Livermore's getter-based hydrogen sensor include (counterclockwise from top) the sensor case; a fiber bundle, consisting of a central laser delivery fiber surrounded by six light-collection fibers; a getter made of 1,4-bis(phenylethynyl)benzene (DEB) and silicone rubber; a spacer ring; and a mirror.

(b) In the assembled prototype, laser light exiting the central fiber passes through the DEB–silicone composite, reflects off the mirror, and makes a second pass through the composite before entering the collection fibers.

The research includes pursuing advanced sensor concepts, such as a gas sensor that can measure material degradation at a parts-per-million level of concentration. One idea is to devise optical methods to monitor chemical processes that produce any type of outgassing. If the researchers can catch outgassing inside a weapon at an early stage, they might be able to identify which material is decomposing or corroding and mitigate the problem quickly. Researchers are also devising methods to extract data from the sensors. One concept involves a portable diagnostics unit that will download sensor data and provide the necessary power sources, lasers, and data-acquisition hardware. To test this concept, the team has developed prototypes that use Raman and infrared spectroscopy as complementary techniques to detect and identify gases. Researchers are also developing a new fiber-based gas sensor, specifically to detect and capture hydrogen. Their design uses photoacoustic Fourier transform infrared spectroscopy to detect changes in an organic material that captures hydrogen. Once embedded in a warhead, the sensor would be fed by infrared laser light supplied through an optical fiber located outside the warhead.

Finally, another project is developing a microelectromechanical systems-based device that uses an array of 120-micrometer-long silicon microcantilevers coated with polymers a few hundred nanometers thick. The polymer swells as it absorbs gas molecules, bending the cantilever and changing its electrical resistivity, thereby signaling the presence of a gas.

Deployed together, networks of these types of embedded sensors could provide valuable information about the weapons in the stockpile much earlier and at much less cost. In so doing, the weapons complex responsible for maintaining the stockpile would be well on the road to transformation. These research efforts were featured in the July/August 2008 issue of ***Science & Technology Review***, an LLNL publication.

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Squeezing out information about "super Earth" planets

A team of Laboratory researchers has developed a new technique to identify phase transitions that may one day reveal the interior structure of so-called "super-Earth" planets. Using one beam of Livermore's Janus laser, the researchers launched a ramp-compression wave, lasting several nanoseconds, against a bismuth sample and measured the telltale signature of a structural phase transformation. Phase transition kinetics describe the time-dependent changes that materials undergo when transforming from one structure to another, whether it's a gas, liquid, solid, or plasma.

Experimental results showed that at the ultrafast time scales of laser-driven ramp-wave-loading, the pressures associated with phase transformations in bismuth increased dramatically compared with previous experiments done on longer time scales. The results suggest that at a critical pressurization rate, the pressure where the phase transition takes place begins to deviate from its equilibrium value. The difference between this observed pressure and the equilibrium phase-transition pressure increased logarithmically with pressurization rate. The research appeared as the cover article in the August 8, 2008 edition of ***Physical Review Letters***.

The experimental platform using laser-driven ramp-wave loading is applicable to pressures relevant to the interiors of recently discovered super-Earth planets, which are several times larger than our own. The technique could help map regions of the structural phase space of materials within these planets, providing critical information for understanding how planets formed and evolved.

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Advanced holographic technique for nanoscale imaging

Livermore and Lawrence Berkeley National Laboratory researchers, along with colleagues from around the world, recently demonstrated the use of x-ray Fourier-transform holography to obtain high-contrast images at the nanoscale. As described in a paper published in the September 2008 issue of ***Nature Photonics***, the use of a uniformly redundant pinhole array next to the sample increased the efficiency of this imaging technique by three orders of magnitude.

The team investigated the technique in two separate experiments. In the first, at the Advanced Light Source at Berkeley, the researchers imaged a lithographically fabricated test sample using a 30-nanometer-thick gold pinhole array with 44-nanometer-square scattering elements. In the second experiment, at the FLASH free-electron laser (FEL) in Hamburg, researchers used 15-femtosecond soft x-ray pulses to image a bacterial cell with a uniformly random pinhole array capable of 150-nanometer spatial resolution. While the high-intensity FEL pulse eventually vaporized the sample and the array, the reconstructed images showed that they remained intact during the exposure. Analysis of the results shows that the massively parallel holographic method produces images that are orders of magnitude more intense than those from conventional Fourier-transform holography, while providing both amplitude- and phase-contrast information. The ultimate spatial resolution obtainable with this technique will depend on future capabilities to fabricate uniformly redundant arrays with larger numbers of smaller (nanoscale) scattering elements. As x-ray lasers move to shorter wavelengths, the team expects to obtain higher-spatial-resolution, ultrafast movies of transient states of matter.

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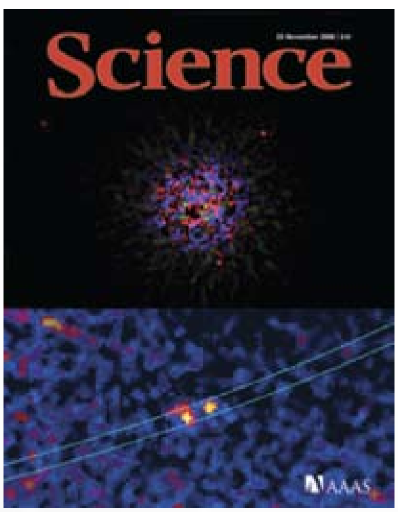
First-ever direct images of a multiplanet extrasolar system

Current and former PLS researchers led a team that reported the first-ever direct images of multiple extrasolar planets orbiting a distant star. High-contrast observations with the adaptive optics systems at the Keck and Gemini telescopes produced images that reveal three planets orbiting the star HR 8799, 130 light years away in the constellation Pegasus. Observations over multiple epochs show counterclockwise orbital motion for all three imaged planets. Their low luminosity and the estimated age of the system imply planetary masses between 5 and 13 times that of Jupiter. This extrasolar system apparently resembles a scaled-up version of the outer portion of our own solar system. These results, which appeared in an article featured on the cover of the November 28, 2008 issue of ***Science***, quickly gained widespread notice. The ***New York Times*** quoted Livermore researcher Bruce Macintosh as saying, “Every extrasolar planet detected so far has been a wobble on a graph. These are the first pictures of an entire system.”

This achievement was made possible by the novel observational technique used by the team. In general, quasistatic speckle artifacts limit the sensitivity of high-contrast ground-based imaging with adaptive optics (AO). The main source of speckles is surface errors on the telescope primary mirror and internal optics. To remove this noise, the researchers used angular differential imaging (ADI), which takes advantage of the rotation of the Earth and the telescopes to distinguish the signal of exoplanets from optical artifacts. An ADI sequence involves keeping the science camera fixed relative to the telescope and allowing the field of view to slowly rotate with time around the star. The team made their observations in the near-IR wavelength region (1.1 to 4.2 micrometers), where the planets are expected to be bright and where the AO system provides excellent image correction.



Livermore researchers are leading the multi-institutional, international collaboration that is developing the next-generation AO instrument for deployment at the Gemini South telescope in Chile in 2010. The primary goal of the Gemini Planet Imager will be to detect more planets (from 1× to 10× the mass of Jupiter) outside our solar system, to provide more information on how planets form and solar systems evolve. GPI's extreme AO system—developed at Livermore—will make it possible to directly observe planets that are now not visible from Earth or from the Hubble Space Telescope, and to spectroscopically study the atmospheres of these extrasolar planets for the first time. GPI will also enable astronomers to investigate the dusty debris disks that surround many stars. Debris disks are old and cold, and therefore have very faint thermal emission. However, scientists can identify them by imaging the light scattered by the dust. Polarization data and high-contrast images will allow astronomers to disentangle dust grain composition, sizes, properties, and their distribution. This will lead to a better understanding of the dynamics of disks and the formation of extrasolar planetary systems.

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Understanding the physics of tokamaks

Livermore researchers are advancing the science underlying the tokamak concept for magnetically confined fusion through collaborations on experiments at the DIII-D Tokamak at General Atomics in San Diego. Results will have important implications for the performance of the International Thermonuclear Experimental Reactor (ITER), a major international project with significant U.S. participation. Recently the Institute of Physics highlighted the 20 most frequently downloaded articles published in ***Nuclear Fusion*** in 2008. Two of these papers described research at DIII-D led by Livermore scientists.

A critical issue for fusion devices is the erosion of the first wall of the experimental device due to impulsive heating from repetitive magneto-hydrodynamic instabilities known as edge-localized modes (ELMs), which occur at the edge of the plasma in a tokamak. In a recent experiment, the researchers demonstrated the suppression of type-I ELMs by applying resonant magnetic perturbations using a single toroidal row of internal, small-aperture coils located either above or below the equatorial plane of the DIII-D tokamak. This feat was accomplished in plasmas, in which some of the plasma characteristics, such as electron collisionality, shape of the magnetic flux surface and edge safety factor, were similar to those expected in ITER. Interestingly, the researchers observed no suppression of the ELMs when they used a single row of external, large-aperture coils on the outer equatorial mid-plane. These results were published in the December 2008 issue of ***Nuclear Fusion***.

The other most frequently downloaded paper, which appeared in the April 2008 issue, reported 3D calculations of the effects of resonant magnetic perturbations on the heat transport in DIII-D plasmas. The simulations show that the heat flux is spread over a wider area of the diverter, thereby reducing the peak heat flux delivered during steady-state operation. The main function of the diverter is to exhaust heat generated by fusion reactions in the plasma core. Since the diverter is the primary interface component between the plasma and material surfaces, it must tolerate high heat loads, which, in some designs, exceed the energy flux through the surface of the Sun. Reducing the heat load would improve the overall performance of tokamaks.

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Chemistry

Unraveling the behavior of detonating explosives

Although high explosives have been used for more than a century, little is known about their microscopic properties during detonation. To improve understanding of this physical process, researchers from Livermore and the Massachusetts Institute of Technology have performed quantum molecular dynamics simulations of a shocked explosive near detonation conditions. The research, which was funded by Livermore's Laboratory Directed Research and Development Program, provides the first "observation," at the molecular level, of material behavior behind a detonation shock wave. The simulation modeled nitromethane, an optically transparent and electrically insulating high explosive that is more energetic than TNT. The results, which appeared in the January 2008 edition of ***Nature Physics***, showed that, behind the shock wave, nitromethane becomes optically reflective and semimetallic for a short time and then transforms back into a transparent, insulating material. The quantum molecular dynamics simulation of nitromethane serves as the first step in understanding molecular properties of shocked explosives at detonation conditions. The researchers are continuing to improve their simulations capabilities with the ultimate goal of being able to calculate the detonation properties of new, yet-to-be synthesized designer explosives.

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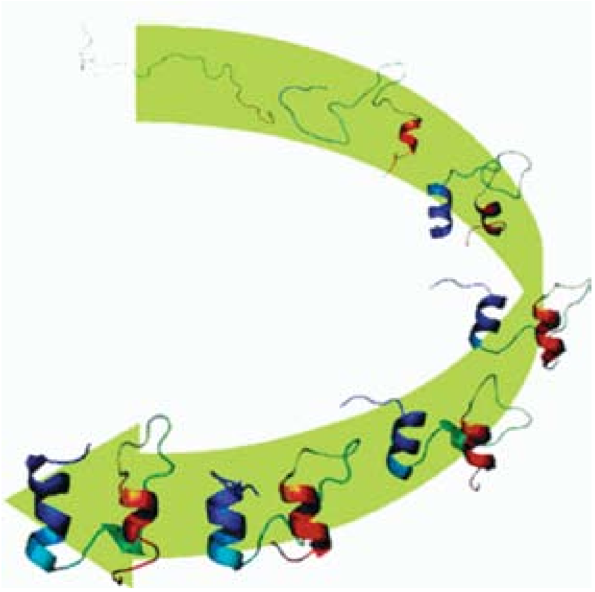
New model for externally forced bond breaking in molecules

A PLS researcher has formulated a new, unified theory to model how an externally applied force can assist the breaking of a chemical bond or the transition from one configuration to another in an individual molecule. Up to now, two well-known but very different theories have been used to describe the temperature-dependent kinetics of such processes, with the attendant debate as to which theory is more appropriate.

The kinetics—the rate of transition from one state of the molecule to another—depend on the energy barrier that the vibrating atoms within the molecule must overcome to make the transition. The increasing external force lowers the energy barrier with time, increasing the kinetics of the transition. In turn, the average force required to drive the transition is sensitive to the loading rate—the change in the strength of the force with time. The researcher derived a model that describes the average force required to drive the molecule from one state to another for all relevant loading rates, thus generating the complete force spectrum. He was then able to show that the two previously used models are just limiting cases, one being valid for low loading rates and the other for high loading rates. His unified model also confirms predictions that, for slow loading rates, forced transitions over single-barrier potentials of virtually any shape can be described by a simple phenomenological model.



Protein folding is one process in which force can assist in changing a molecule from one state to another. In this case, after an initial collapse into a globular state, the 1BBL protein continues to fold until it reaches its final native structure.

To demonstrate the validity of the unified theory, the researcher applied it to experimental data for forced barrier crossings in two different systems. One of the systems consisted of biotin—i.e., vitamin B7, a cofactor in the metabolism of fatty acids—and avidin, a protein that binds to biotin with a very high affinity. For the forced rupture of the biotin–avidin chemical bond, his model fit the experimental force spectrum remarkably well over the more than million-fold range of loading rates explored in the experiment. The extracted energy barrier height of 4.93 ±0.23 kilocalories per mole and transition state of 3.07 ±0.22 angstrom matches very well with the energy surface rigorously reconstructed from the same experimental data. This research appeared in the April 4, 2008 issue of the ***Physical Review Letters***.

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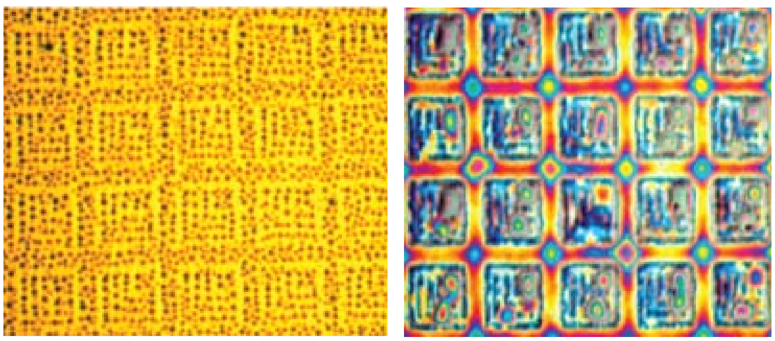
Photocatalytic lithography applied to life sciences

Livermore researchers and their collaborators at Monsanto Company in St. Louis and the Swiss Federal Institute of Technology in Lausanne, Switzerland used innovative photocatalytic techniques to pattern proteins and cells to demonstrate their utility in life science applications. The research appeared in the May 6, 2008 edition of ***Langmuir***, published by the ***American Chemical Society.*** Photocatalytic lithography couples light with photoreactive, coated mask materials to pattern surface chemistry. The researchers excited porphyrins as the photosensitizer to create radical species that photocatalytically oxidized, and thereby patterned, chemistries in the local vicinity. Advantageously, the technique does not require photoresist; is inexpensive, fast, and robust; primarily operates in the molecular, as opposed to the physical, domain; and can accommodate various mask materials, chemistries, and substrates. The wavelength of light does not limit the resolution of patterned features.

To demonstrate the technique, the researchers photocatalytically patterned silane using porphyrins and then covalently grafted a non-fouling background to the remaining silane. They analyzed the patterned substrates using atomic force microscopy and time-of-flight secondary ion mass spectrometry. They also exposed the patterned surfaces to protein and cells and found that protein adsorption and cell adhesion was restricted to the patterned regions, which had been modified with an adhesive chemistry. This result confirmed the robustness of the patterning technique.

While the initial research involved micrometer-scale patterning features, the team is working to expand the technique to the nanoscale. They presently can pattern arbitrary features with line widths of 200 nm and aspect ratios up to 160:1.



(left) The patterned silicon substrate formed by selectively removing silane from regions subjected to reactive oxygen species generated from the excited photosensitizer. (right) The hydrated silicon surface after grafting a thin (~15-nm) polymeric hydrogel layer onto the remaining silane.

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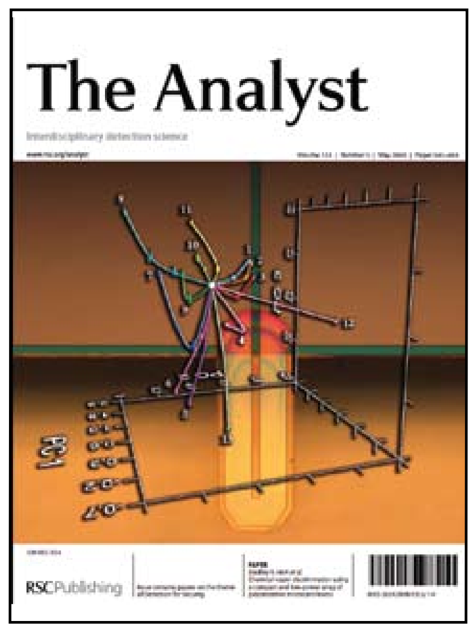
New sensor for analyzing chemical vapors

A paper by Lawrence Livermore researchers describing the development of a compact, low-power sensor array to detect chemical vapor analytes was chosen as the cover article of the May 2008 issue of the ***Analyst***—devoted to detection for security. The researchers demonstrated the use of the sensor array to detect 11 chemical vapors representing a breadth of chemical properties, in real time and over a wide range of vapor concentrations. They also reported, for the first time the detection of the chemical warfare agents VX and sulfur mustard using a polymer-based cantilever sensor array. The eight-cantilever sensor array has shown sensitivities from 4 parts per billion to 16 parts per thousand in 13 chemicals ranging from water to volatile organic compounds, whose industrial emissions are regulated because of their deleterious health effects. Slightly larger than a matchbook, the system can fit unobtrusively in small spaces. It is a candidate for use in a Homeland Security Advanced Research Projects Agency initiative that seeks technology to integrate sensors for chemical, biological, or radiological threats onto a mobile communications platform, such as a cell phone. Such a network would warn of, identify, and detect the scope of a potential threat agent.



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Broad-spectrum detection of hazardous aerosols

Livermore researchers have demonstrated that a single-particle aerosol mass spectrometry (SPAMS) system can rapidly detect and identify actual or surrogate chemical, biological, radiological, nuclear, and explosive materials and illicit drug precursors in aerosol form. The system performs not only the sampling of such aerosols but also the physical analysis and subsequent data processing required to generate highly reliable alarms. In a paper published in the June 15, 2008 issue of ***Analytical Chemistry***, the researchers describe a laboratory experiment involving actual threat and surrogate releases mixed with ambient background aerosols that demonstrated accurate broad-spectrum threat detection in seconds. Data from a field test at the San Francisco International Airport further demonstrated the system's capability for extended field operation with an ultralow false alarm rate.

Together, these results demonstrate a significant advance in rapid aerosol threat detection. The SPAMS technology was highlighted as a "notable development in chemistry" in the Editor's Choice section of the June 20, 2008 issue of ***Science***.

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Bioterrorism instrument adapted to detect tuberculosis

An instrument originally designed for detecting the malicious use of biological pathogens has a potential application in the public health sector—to rapidly screen for tuberculosis. In experiments over the past year, a Livermore research team has used single-particle aerosol mass spectrometry (SPAMS) to detect a tuberculosis surrogate, even when surrounded by sputum and mucuslike substances. The team was also able to differentiate two similar bacteria, distinguishing an avirulent strain of tuberculosis from *Mycobacterium smegmatis*. This is an important finding because many bacterial infections cause tuberculosis-like symptoms. The team's research, which was funded by Livermore's Laboratory Directed Research and Development Program, was published in the July 15, 2008 issue of ***Analytical Chemistry***.

With current methods, diagnosing tuberculosis can be difficult and expensive. The "gold standard" method is to culture samples, a process that can require days to weeks. While waiting for cultures to grow, medical personnel may release patients, allowing them to infect the general public. In addition, valuable resources may be wasted when unneeded precautions, such as chest x rays or patient isolation, are taken for people who, in the end, do not have the disease. Health-care providers and emergency response personnel need a method to differentiate the infections within minutes. The Livermore team's results suggest that SPAMS could potentially fill this need by detecting tuberculosis in concentrated samples. However, many challenges remain before this potential can be realized in routine testing of patients in clinical settings. The challenges include understanding patient-to-patient variations in background lung matrix (sputum) and number of tubercle bacilli; detection thresholds and sensitivities for discriminating virulent tuberculosis, virulent tuberculosis confounders, near-neighbor bacteria, and natural mutations of virulent tuberculosis; and development of a suitable human sample interface.

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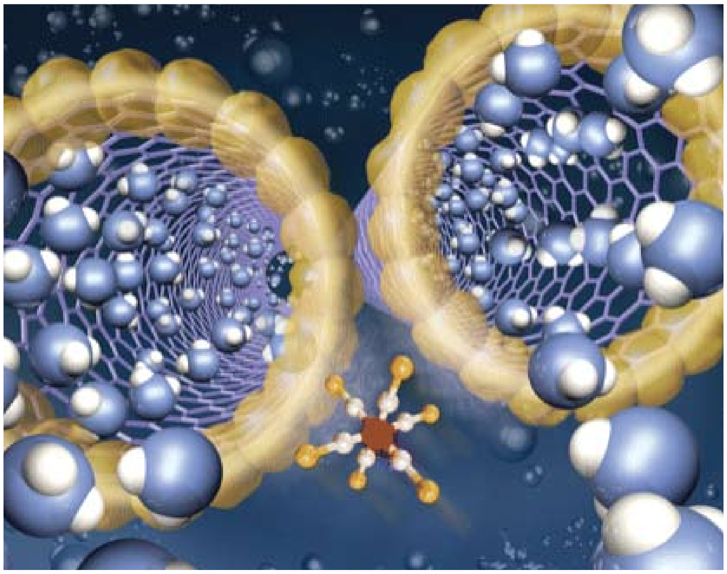
Advances in understanding the functionality of carbon nanotubes

PLS scientists have continued to investigate the properties and functionality of carbon nanotubes. Because of the potential application of nanotube-based membranes to water filtration in desalination and biological research, their results have gained widespread recognition in the scientific community and in the press.

In a paper published in the July 2008 edition of ***Nano Letters***, a team of researchers from Livermore and the University of North Carolina reported the positive identification of water confined in the interior of single-walled carbon nanotubes (SWCNTs). By using controlled experiments with both sealed and opened SWCNTs, and by independently measuring the interior water content through desorption experiments, the researchers were able to distinguish the proton nuclear magnetic resonance signals from confined and exterior water molecules. With this technique, scientists will be able to probe the detailed dynamics of water flow through carbon nanotubes. Shortly after its online publication, this paper was highlighted by United Press International.



Mimicking the biological pore aquaporin, carbon nanotubes with negative charges on their rims exclude ions such as ferricyanide while selectively transporting water at a high rate.

In another paper, published as the cover article of the November 11, 2008 edition of the ***Proceedings of the National Academy of Sciences***, a PLS team reported their investigation of ion transport through carbon nanotube pores. For these experiments, the researchers used a nanofluidic platform consisting of a silicon nitride membrane and, as pores, aligned carbon nanotubes less than 2 nanometers in diameter. They used a plasma treatment to introduce the negatively charged groups at the opening of tubes. Pressure-driven filtration experiments, along with capillary electrophoresis analysis, provided quantitative data on ion rejection by the membrane as a function of pH, solution ionic strength, and ion valence. The results showed significant ion rejection that can be as high as 98%. Shortly after its online publication, this paper was highlighted in the June 23 edition of ***Chemical and Engineering News*** and in a ***ScienceDaily*** newsletter.

An earlier Livermore publication, entitled “Fast mass transport through sub-2-nanometer carbon nanotubes,” which was featured on the cover of the May 19, 2006 edition of ***Science***, was the most highly cited paper in chemistry during the March–April 2008 period according to ***Science Watch***.

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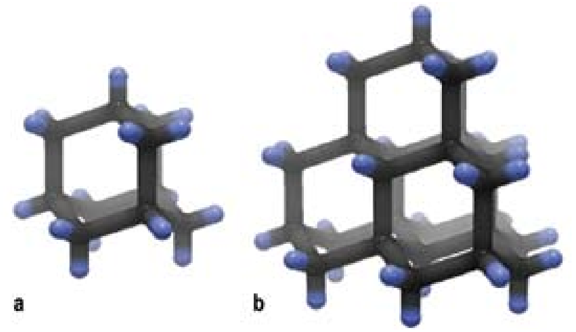
Novel properties and use of diamondoids

For many years, tiny diamondlike particles, equivalent to a billionth of a billionth of a carat, have plagued oil workers when the particles clump together and clog pipelines. These particles, called diamondoids, can be found in crude oil at concentrations up to thousands of parts per million. At the atomic level, diamondoids consist of hydrocarbon molecules with cubic-diamond-cage structures, and their properties depend on the number of cages or units in the structure. Similar diamondlike carbon nanoparticles occur in meteorites, interstellar dust, and protoplanetary nebulae. High-explosive detonations have produced much larger, less pure diamond nanoparticles. Livermore researchers have been working, in collaboration with scientists from other institutions and Chevron Corporation, to transform diamondoids from pesky pipeline sludge and astronomical curiosity into building blocks for new materials. They have also been investigating the microscopic particles’ fundamental structural, electrical, and optical properties, which could lead to new applications in nanotechnology.



(a) Adamantane consists of 10 carbon (black) and 16 hydrogen (blue) atoms. Diamondoids form when multiple adamantane units, or cages, join together. (b) Pentamantane (five units) can be viewed as one adamantane cage surrounded by four additional cages.

Recently, the researchers have studied the properties of self-assembled monolayers (SAMs) of diamondoids on gold. In particular, they have used near-edge x-ray absorption fine structure spectroscopy and x-ray photoelectron spectroscopy to determine the effects of substituting a thiol group on the orientation and electronic properties of the diamondoids composing the monolayer. Analysis of the experiments revealed highly ordered SAMs, with the molecular orientation controlled by the location of the thiol group. The electronic binding energies in the carbon and sulfur atoms varied with diamondoid monolayer structure and thiol substitution position, consistent with different degrees of interaction with the gold substrate. This research, published in the August 13, 2008 edition of the ***Journal of the American Chemical Society***, demonstrates control over the assembly, in particular the orientational and electronic structure, providing a flexible design of surface properties with this class of diamond nanoparticles.

Within a few years, diamondoids could be used in products ranging from electron microscopes to pharmaceuticals, to fuel additives and material coatings. In the growing world of nanotechnologies, diamondoids will likely play an important role as adaptable building blocks for new materials with novel properties.

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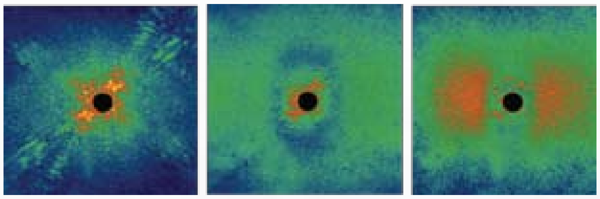
Materials Sciences

Snapshots of a solid taken on ultrafast time scales

Laboratory researchers, along with colleagues from around the world, have captured time-series snapshots of a solid as it evolves on ultrafast time scales. Using the soft x-ray free-electron laser (XFEL) at the Deutsches Elektronen-Synchrotron Research Centre in Hamburg, Germany, the team observed, with nanometer-scale spatial resolution, the condensed-phase dynamics of a sample as it undergoes laser ablation. Results from this research appeared in the July 2008 issue of ***Nature Photonics***.



Evolution of the laser-heated sample revealed by coherent x-ray diffraction. Measured, single-shot diffraction patterns at –5 ps (left), corresponding to the object just before the excitation pulse. The diffraction patterns from the same object at 15 ps (middle), and 40 ps (right) after the excitation pulse. Gradual degradation of the nanofabricated sample is shown by the loss of high spatial frequency information in the diffraction patterns. The pump laser is linearly polarized with the electric-field vector oriented vertically with respect to these images.

The researchers used an optical laser pulse to heat the solid target. They used 10-femtosecond-long pulses of x rays from the XFEL to probe the ablating target by means of coherent diffraction. By varying the time delay between the optical and x-ray pulses, they were able to obtain a time series with a 50-nanometer spatial resolution and a 10-picosecond temporal resolution. The “shutter speed” of the diagnostics, which is determined by the duration of the x-ray pulse, allows the team to observe events occurring at the atomic level before the sample is completely destroyed.

The ability to take images in a single shot is key to studying nonrepetitive, dynamic behavior in a sample. With the new technique, researchers will be able to study the ultrafast dynamics occurring in noncrystalline materials under extreme conditions, such as fracture, shock, and plasma formation, as well as slower processes in the solid state, such as nucleation and phase growth, phase fluctuations, and various forms of electronic or magnetic segregation.

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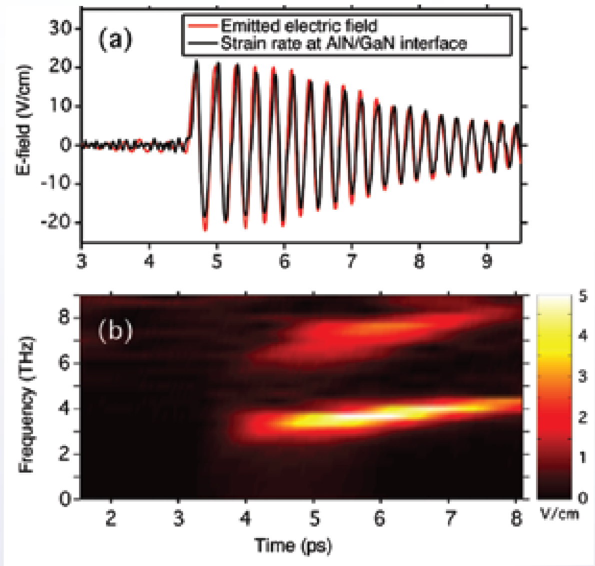
New form of coherent radiation generated in solids

PLS researchers and their collaborators from Los Alamos National Laboratory demonstrated that acoustic strain waves in a solid can generate a new form of detectable coherent radiation, which contains sufficient information to directly determine the time dependence of the stress or strain in the wave with picosecond resolution. Using molecular dynamics simulations and analytics, the team found that the radiation is generated when strain waves with terahertz frequencies propagate past an interface between materials with different piezoelectric coefficients. For the specific case of aluminum nitride–gallium nitride (AlN–GaN) heterostructures, when a shock wave passes the interface, stress waves with frequencies up to eight terahertz can form spontaneously in the material. Polarization currents generated by the high-frequency strain waves at the interface lead to emission of radiation at the frequencies associated with the strain waves. Knowledge of the high-pressure optical properties of the materials being probed is not required for the interpretation of this phenomenon, as is often the case.

The team used nonequilibrium molecular dynamics (MD) simulation to investigate the propagation of a shock in wurzite structure GaN, which is a hard material capable of withstanding large stresses without undergoing irreversible plastic deformation of the crystal lattice. Large amplitude oscillations form spontaneously at the shock front and increase in number as the wave propagates. The amplitude of these terahertz oscillations are significantly larger (by a factor of 30) than those observed in recent experiments. However, shock waves with such large strain amplitudes could be generated experimentally using a sub-picosecond laser pulse with a millijoule or greater energy. MD simulations of an AlN–GaN interface show that the time dependence of the electric field produced is closely related to the strain rate at the interface, suggesting that the resulting radiation could be used to directly probe terahertz-frequency strain waves. This research appeared in the July 4, 2008 issue of ***Physical Review Letters***.



(a) Comparison of the strain rate to the electric field taken at 1 millimeter from the interface in a molecular dynamics simulation of a shock wave passing through the aluminum nitride–gallium nitride interface. The time dependence of the electric field is closely related to the strain rate at the interface, enabling direct resolution of terahertz frequency strain waves. (b) Frequency as a function of time for the electromagnetic radiation. The 8 THz harmonic of the 4 THz fundamental frequency, visible in the image, corresponds to atomic-scale spatial structure of about 0.5 nanometer.

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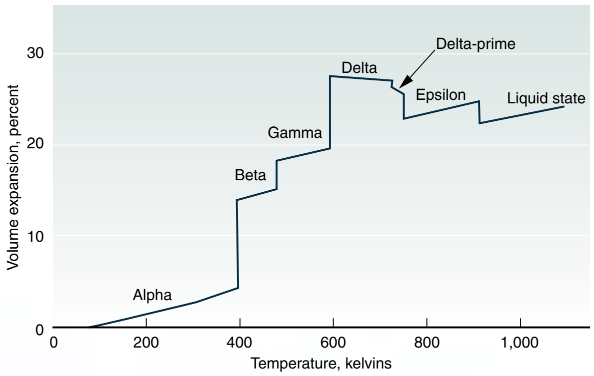
Simulations give new insight into the properties of plutonium

Plutonium, in addition to being one of the most important elements to the Laboratory's missions, is also arguably one of the most complex elements known—with six phases in its solid state. To the Laboratory, the most important phase is the delta phase, in which plutonium is most malleable.



As temperature increases, plutonium's volume changes dramatically before it becomes a liquid. The radioactive metal is unique among elements in exhibiting six solid phases at ambient pressure.

In an effort to explain some of plutonium's unusual properties and better understand results from past experiments, PLS scientists and their collaborators from Rutgers University used the Laboratory's Atlas supercomputer to perform some of the most precise simulations yet of delta-phase plutonium. For these simulations, the team combined density functional theory and dynamical mean field theory (DMFT) to calculate the delta phase's electronic structure and its almost complete lack of magnetism. The researchers leveraged recent advances in the continuous-time quantum Monte Carlo method to achieve, for the first time ever, an exact solution of the effective impurity problem generated by DMFT. The simulations predict that, at room temperature with delta-phase plutonium at its equilibrium volume, the f electrons are delocalized—they easily move about the lattice of plutonium atoms and are not associated with one particular atom. As the lattice expands, the f electrons become localized—that is, they are more associated with one particular atom and thus cannot easily hop through the lattice. The transition from delocalized to localized behavior occurs at increasingly lower temperatures as the lattice volume increases. With greater distance between the electrons, delta-phase plutonium begins to behave more like other materials with strong electron correlation. Calculation of the magnetic susceptibility indicates Pauli-like behavior—weakly paramagnetic itinerant electrons—at the equilibrium volume of delta-phase plutonium, in support of experimental measurements. Expanding the volume causes the electrons to cross over from delocalized to localized behavior at increasingly lower temperatures, which manifests itself in Curie-like behavior of the magnetic susceptibility—increasing susceptibility with decreasing temperature, consistent with measurements in plutonium hydride. This research appeared in the August 1, 2008 issue of ***Physical Review Letters.***

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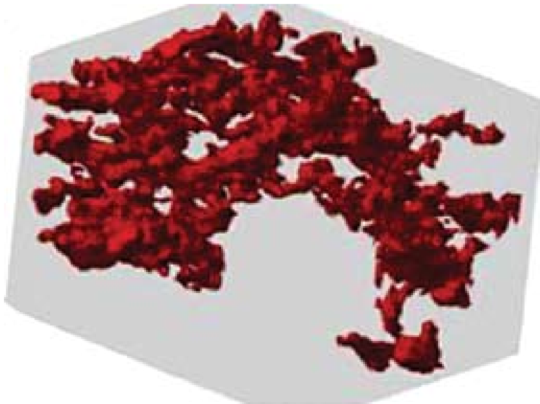
Scientists improve understanding of aerogel with 3-D images

Scientists from Livermore and Lawrence Berkeley National Laboratories have created three-dimensional images of an aerogel to determine its bulk structure and strength, and to identify potential new applications. Aerogels are engineered materials designed for a high strength-to-weight ratio, which exhibit astonishing mechanical, thermal, catalytic, and optical properties because of their low density and porous structure. In the August 1, 2008 issue of ***Physical Review Letters***, the researchers reported the use of x-ray diffractive imagining to obtain high-resolution views of the labyrinthine internal structure of a tantalum oxide nanofoam aerogel. Using data obtained at the Advanced Light Source at Lawrence Berkeley National Laboratory, the team inverted coherent x-ray diffraction patterns to capture the three-dimensional bulk lattice arrangement of a micrometer-sized piece of aerogel with a density of 0.1 gram per cubic centimeter. The results show a structure consisting of bulbous nodes connected by thin beams. These are similar to the fractal cluster aggregates and links derived from a diffusion-limited cluster aggregation model. The resultant three-dimensional model also agreed with small-angle x-ray scattering measurements made at the Advanced Photon Source at Argonne National Laboratory.



Section and isosurface rendering of a 500-nanometer cube from the interior of the imaged sample of aerogel. The foam structure shows globular nodes that are interconnected by thin beamlike struts. Approximately 85% of the total mass is associated with the nodes.

The blob-and-beam structure explains why these low-density materials are weaker than predicted. Thinning of the measured structure in finite-element simulations improves the strength-to-weight ratio by orders of magnitude. This suggest that improvements in the strength of this aerogel could be obtained by modifying the preparation conditions in an effort to redistribute constituent material from the nodes to the interconnected struts.

In the past, Livermore researchers have developed and improved aerogel for national security applications, synthesized electrically conductive inorganic aerogel for use as super-capacitors, engineered aerogel as a water purifier to extract harmful contaminants from industrial waste or to desalinize seawater, and used aerogel to capture cometary dust particles by NASA's Stardust spacecraft.

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New electron microscope takes nanosecond snapshots of materials

In a paper published in the September 12, 2008 issue of ***Science***. PLS researchers described their in situ observations of the moving reaction front of a reactive multilayer foil. The team initiated the self-sustaining exothermic reaction with a pulsed laser, which heated a small portion of the foil. They used a photo-emitted electron pulse to probe the dynamics with "snapshot" diffraction and imaging with 15-nanosecond resolution inside a dynamic transmission electron microscope (DTEM). The time delay between the laser and electron pulses could be precisely controlled within a range from nanoseconds to hundreds of microseconds, with a timing jitter of 1 nanosecond. Time-resolved images and diffraction showed a transient cellular morphology in a mixing, self-propagating reaction front, and revealed brief phase separation during cooling. These results provide new insights into the mechanisms driving the self-propagating high-temperature synthesis. The team also compared the images of the high-temperature reaction front obtained with both fast optical imaging and with the DTEM. In addition to the significantly higher resolution of the DTEM, analysis of the associated electron diffraction data allowed determination of changes in the crystal structure, and hence the temporal phase behavior of the reactive material. These results clearly showed that DTEM is capable of the direct nanoscale characterization of irreversible, dynamic phenomena occurring on the time-scale of tens of nanoseconds.

Since the invention of the first TEM in 1938, scientists gradually improved its maximum spatial resolution to better than 0.1 nanometer but had less success at improving the TEM's temporal resolution. Livermore's DTEM is the only technology available for generating direct nanometer-resolution images of irreversible events at time scales ranging from 15 nanoseconds to milliseconds. The researchers are currently developing the next-generation instrument, which will be able to take several consecutive images, creating a movielike record of microstructural features as they rapidly evolve in time. With such an extended capability, DTEM may also serve as a new tool in biological research, enabling scientists to observe a biological function in action. This would allow them to analyze the changing structures of chromosomes, membrane proteins, and other biomolecules, or the cellular activities occurring in processes such as mitosis.

The dynamic transmission electron microscope (DTEM) captures nanoscale images a million times faster than conventional instruments.

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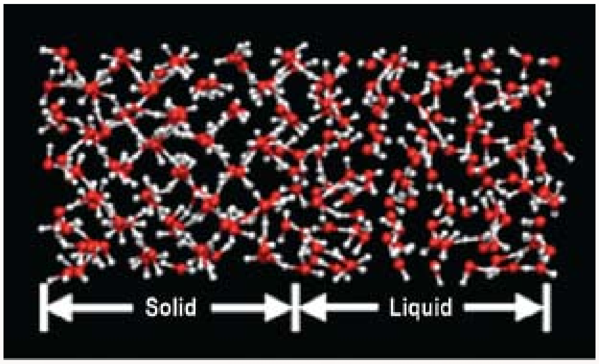
Melting ice under pressure

A team of scientists from the Laboratory and the University of California at Davis performed first-principles molecular dynamics simulations using a two-phase approach to determine the melting temperature of ice VII (a high-pressure phase of ice) at pressures ranging from 100,000 to 500,000 atmospheres. The researchers found that, for pressures up to 400,000 atmospheres, ice melts as a molecular solid. For higher pressures, the melting curve—the melting temperature as a function of pressure—increases sharply because of the presence of molecular dissociation and proton diffusion in the solid prior to melting. The simulations also show that the onset of significant proton diffusion in ice VII as a function of increasing temperature is gradual and bears many similarities to that in a type II superionic solid.

The team's results elucidate the melting curve at extremely high pressures (from 350,000 to 450,000 atmospheres), similar to those found in the interiors of Neptune, Uranus, and Earth. Determining the melting curve of water is important in many scientific fields, including physics, chemistry, and planetary science. Researchers have proposed that the cold subduction zones in Earth are likely to intersect with the high-pressure melting curve of water. If accurate, this hypothesis would have profound implications for the composition and transport of materials in the interior and the long-term evolution of the planet as it cools. The team's results appeared in the September 23, 2008 edition of the ***Proceedings of the National Academy of Sciences***.



Representation of the atoms [oxygen (red) and hydrogen (white)] taken from a quantum molecular dynamics simulation of the two phases of water at a pressure of 500,000 atmospheres. The coordinates of the atoms correspond to the initial starting configuration at 2,000 kelvin showing a clear demarcation between ice and liquid water.

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Shedding light on phase transition in cerium

Using accurate x-ray diffraction measurements, a team of PLS physicists determined the previously disputed location of the critical point associated with the gamma–alpha phase transition in cerium, a lanthanide metal that exhibits unusual behavior at high pressures. In particular, an isostructural volume collapse—large decrease in volume—occurs under compression at the gamma–alpha phase transition. The magnitude of the volume collapse decreases with increasing temperature, and eventually terminates at the critical point. The underlying physical mechanism has been controversial but is thought to be associated with dramatic changes in the behavior of the 4f electrons, either a Mott transition or a significant change in the screening of the magnetic moments (Kondo model). Data from the new Livermore experiments locate the critical point at 1.5 gigapascals and 480 kelvin, resolving previous controversies. The researchers find that the data, as a function of pressure and temperature, can be well fitted by the Kondo volume collapse model augmented with a quasi-harmonic treatment of the lattice vibrations.

The research team used the HPCAT beam line of the Advanced Photon Source at Argonne National Laboratory to obtain angle-dispersive x-ray diffraction patterns of cerium as function of pressure and temperature. The samples were enclosed in an externally heated diamond anvil cell. Diffraction data were generated between room temperature and 800 kelvin, and pressures up to 5 gigapascals. The measured isotherms—volume as a function of pressure at constant temperature—clearly identify the critical point at 480 kelvin, as no phase transition or volume collapse is observed at temperatures above this value. This research appeared in the October 17, 2008 edition of ***Physical Review Letters***.

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Electronic structure of plutonium elucidated

PLS scientists have used density-functional theory calculations with the mixed-level and magnetic models to study the electron configuration in plutonium. By combining the computational results with data from photoelectron spectroscopy, synchrotron radiation-based x-ray absorption measurements, and electron energy-loss spectroscopy, they found that the number of electrons in the 5f orbital is between 5 and 6—contrary to what has recently been suggested in several other publications. The Livermore team treated the 5f electrons relativistically and constrained the spin magnetic moment so that the spin and orbital magnetic moments exactly canceled each other. To test this approach, they generated a simulated photoelectron spectra and compared it to the to extant experimental spectrum for delta plutonium–gallium. By combining the spin and orbital specific densities of states with state, spin, and polarization depended transition moments, the researchers were able to reconstruct the experimentally observed spectra from delta plutonium–gallium obtained with linearly polarized soft x-rays, thus directly confirming the validity for their approach. Because this agreement is a necessary but not sufficient condition for demonstrating the correctness of their model, the researchers propose a new experiment—Fano spectroscopy—to resolve conclusively the controversy surrounding the electronic structure of plutonium. This research appeared in the March 26 and October 22, 2008 editions of the ***Journal of Physics: Condensed Matter.***

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Improved understanding of amorphous materials

A team of researchers from Lawrence Livermore and Lawrence Berkeley National Laboratories and Rutherford Appleton Laboratory in the United Kingdom developed a new method that provides improved models of the atomic and void structures of network-forming elemental materials. Applications of the method could revolutionize the process of creating new solar panels, flat-panel displays, optical storage media, and myriad other technological devices.

The researchers used x-ray diffraction of amorphous red phosphorus compressed to 6.30 gigapascals, supplemented with micro-Raman scattering studies, to build three-dimensional (3D) structural models consistent with the diffraction data. They discovered that the pressure dependence of the first sharp diffraction peak intensity and line position can be quantitatively accounted for by a characteristic void distribution function, defined in terms of average void size, void spacing, and void density. They also created 3D models of pressure-dependent structures of amorphous red phosphorus that for the first time are accurately portrayed by neutron and x-ray diffraction studies. The researchers also developed a new method to accurately characterize void structures within network-forming materials.

In the 1970s and 1980s, amorphous or disordered materials were found to exhibit technologically viable properties for use in photovoltaic cells and portable optoelectronic storage media such as CDs, DVDs, and more recently Blu-Ray disks. However, attempts by scientists to accurately characterize seemingly simple elemental materials such as amorphous red phosphorus were hindered because the appropriate analysis tools simply did not exist. The diffuse scattering analysis tools developed by these scientists will enable more systematic engineering routes for designing and characterizing amorphous materials. The mechanical, optical, magnetic, and electronic plasticity of amorphous materials hold great promise for enhancing current and emerging technologies. The research appeared in the November 2008 edition of ***Nature Materials***.

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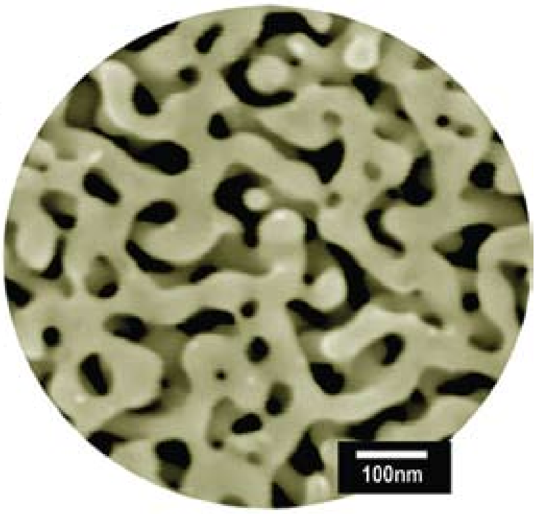
Mechanical response without heat or electricity

Laboratory researchers in collaboration with the Institut für Angewandte und Physikalische Chemie of the Universität Bremen and the Institut für Nanotechnologie of the Forschungszentrum Karlsruhe (both in Germany) have found a new method that directly converts chemical energy into a mechanical response without generating heat or electricity first. The team took a sample of nanoporous gold and alternately exposed it to ozone and carbon monoxide. Using the oxidation of carbon monoxide by ozone as a driver, the team achieved reversible macroscopic strain amplitudes of up to 0.5 percent. The experiment is based on chemistry-induced changes of the surface stress at a metal–gas interface, which in turn cause the sample to contract and expand. Apparently, this surface-chemistry actuator directly converts chemical energy into a mechanical response without generating heat or electricity first.



Scanning electron micrograph showing the characteristic sponge-like, open-cell morphology of nanoporous gold. The horizontal bar corresponds to a distance of 100 nanometers.

The team selected nanoporous gold for several reasons. It has remarkable catalytic properties and can sustain high stresses. In addition, its open-cell foam morphology allows for mass transport. The research showed that ozone exposure leads to oxygen absorption, which triggers sample contraction by modifying the surface stress. Exposure to carbon monoxide then restores the original sample dimensions by removing the absorbed oxygen. Using molecular dynamics simulations, the team independently verified the effect of surface stress on the equilibrium shape of nanoporous gold and its structural building blocks.

These results, which appeared in the November 30, 2008 online edition of ***Nature Materials***, could lead to the development of a new generation of chemically driven sensors and actuation devices.

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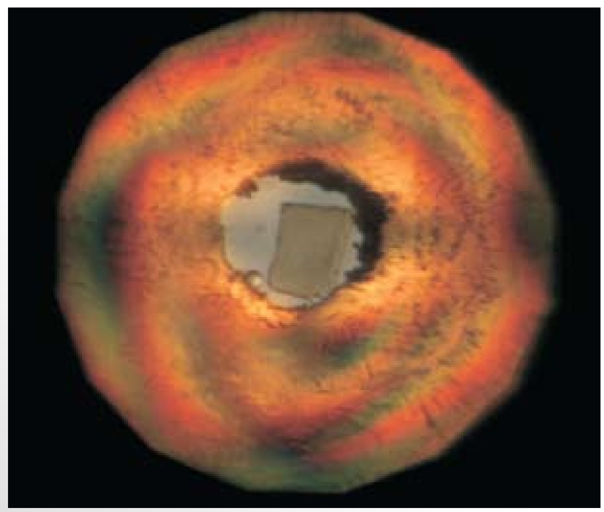
Earth Sciences

New insight into the geophysical structure of deep Earth

Livermore scientists and collaborators from the University of Washington, the Carnegie Institution of Washington, and Northwestern University are working to better understand the seismic structure of deep Earth by examining the elastic behavior of iron-containing minerals under extremely high pressures. The researchers have determined experimentally for the first time the complete elastic tensor of ferropericlase, an iron magnesium oxide found in Earth's lower mantle, through the high-to-low-spin electronic transition induced by high pressures.

The lower mantle comprises more than half of Earth's volume and is subject to extremely high pressures and temperatures. Pressure directly affects the electronic configuration of iron in mantle minerals, such as ferropericlase. Iron exists in the high-spin electronic state at low pressure but changes dramatically to the low-spin state under extreme pressure. The team found that this transition causes ferropericlase to soften in the pressures range from 40 to 60 gigapascals. Although the spin transition is too broad to produce an abrupt seismic discontinuity in the lower mantle, the transition will produce a correlated negative anomaly for both compressional and shear velocities, which extends throughout most, if not all, of the lower mantle. These results, which appeared in the January 25, 2008 edition of ***Science***, will help scientists to test and refine geophysical models, and to improve their understanding of the lower mantle, a deep, inaccessible region of the Earth.



Ferropericlase sample seen through one of the diamonds of the diamond anvil cell at a pressure of approximately 40 GPa (400,000 atmospheres). The sample is surrounded by the pressure medium and rhenium metal gasket.

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Human activities may shape California climate

Through research funded by the California Energy Commission, scientists from the Laboratory, the University of California at Merced, and the National Center for Atmospheric Research found that temperatures in California from 1915 to 2000 have increased by 1.16°C (2.1°F) statewide. The research, which appeared in the March 2008, Supplement 1 edition of ***Climatic Change***—dedicated to California's climate—also suggests that the warming may be related to human activities.

The team used data from nine sets of observational records and from a suite of climate model simulations of natural internal climate variability to analyze trends in California-average temperatures during the periods 1950–1999 and 1915–2000. The researchers found large increases in mean and maximum daily temperatures in late winter and early spring, as well as increases in minimum daily temperatures from January to September. These trends are inconsistent with model-based estimates of natural internal climate variability, and thus require one or more external forcing agents to be explained. The researchers suggest that the warming of Californian winters over the twentieth century is associated with human-induced changes in large-scale atmospheric circulation. Recent climate models have not been effective in explaining California's summertime trend, where warming mainly occurs at night. Based on their previous research, the team suggests that lack of a detectable increase in summertime maximum temperature arises from a cooling associated with large-scale irrigation, which may have counteracted warming from mounting greenhouse gases and urbanization. If this hypothesis is verified, the acceleration of carbon dioxide emissions combined with a leveling of irrigation may result in a rapid summertime warming in the Central Valley in the future.

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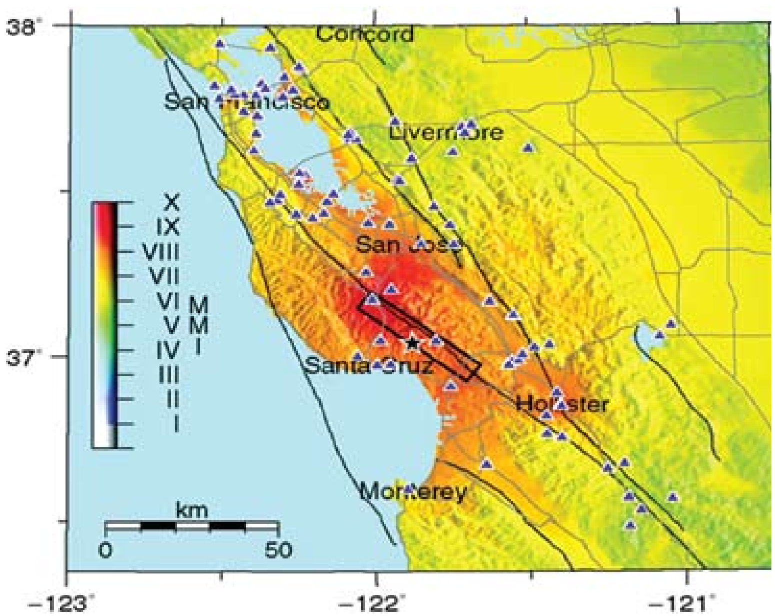
Improved prediction of ground motion in earthquakes

PLS scientists are working to better understand how the ground will respond to the strong forces of an earthquake. In collaboration with the U.S. Geological Survey (USGS), the University of California at Berkeley, and URS Corporation, the researchers have developed improved high-performance computing models that animate ground motion as waves moving outward, color-coded by intensity. The research appears in three papers published in the April 2008 edition of the ***Bulletin of the Seismological Society of America*** on the 102nd anniversary of the 1906 San Francisco earthquake, which ruptured along the San Andreas Fault.



Map of the measured ground motion (peak velocity and acceleration) obtained from seismic networks for the 1989 Loma Prieta earthquake. The star identifies the epicenter, the thick black lines delineate the projection of the fault plane in the source model, and the triangles show locations of the stations used in the construction of the map.

For the first study, the researchers used high-fidelity seismic data from a series of San Francisco Bay Area earthquakes to evaluate a new three-dimensional (3D) geologic and seismic model created by the USGS. Using observations from a network of seismic stations that record broadband data in the region, the team compared computed seismograms with observed recordings for 12 moderate quakes. The team found that, for the 2000 Yountville earthquake, the reported source parameters accurately reproduce the observations at two monitoring stations experiencing strong motion (approximately 10 km from the epicenter). Comparison of the observed and synthetic seismograms shows that the 3D model consistently predicts energy arriving earlier than is observed, particularly for the surface waves. Generally, the results indicate that the 3D model predicts the observed waveforms well and includes features that arise from the interaction of the waves with 3D structure, especially the major sedimentary basins in the San Francisco Bay Area. These findings indicate that the overall structure of the USGS 3D model is accurate, but the velocities in the upper crust must be reduced to improve the predicted timing of surface-wave arrivals.

In the second study, the researchers used four different wave-propagation codes and the 3D geologic and seismic model developed by the USGS to characterize how well the ground-motion simulations reproduced the seismograms recorded during the 1989 Loma Prieta earthquake, which also ruptured along the San Andreas Fault. All of the simulations generated ground motions consistent with the large-scale spatial variations in shaking associated with rupture directivity and the geologic structure. The long-period simulations, on average, underpredicted shaking intensities by about 0.5 units. Discrepancies with observations arise due to errors in the source models and geologic structure. The consistency in the calculated waveforms across the different codes using the same source model suggests the uncertainty in the source parameters tends to exceed the uncertainty in the seismic velocity structure. Based on these findings, the researchers concluded that the 3D seismic velocity model and the wave-propagation codes are suitable for modeling the 1906 earthquake and scenarios of future events in the San Francisco Bay Area.

In the third study, the team used the wave-propagation code E3D to estimate the ground motion that occurred in Central and Northern California during the 1906 earthquake and that might occur in hypothetical earthquakes along the San Andreas Fault. Team members ran the simulations on three Livermore computing systems and the Earth Simulator supercomputer in Japan. The simulations successfully reproduced the main features of the previously compiled Shake Map, but overestimated the intensity of shaking by 0.1–0.5 units. The simulations show that rupture directivity exerts the strongest influence on the variations in shaking, although sedimentary basins consistently contribute to the response in some geographic locations. These findings suggest that future large earthquakes on the northern San Andreas fault may subject the San Francisco Bay urban area to stronger shaking than a repeat of the 1906 earthquake. Ruptures propagating southward towards San Francisco appear to expose more of the urban area to a given intensity level than do ruptures propagating northward. A better understanding of ground motion during earthquakes will help policy makers develop regulations to enhance public safety and emergency response and will lead to improved engineering designs for future construction.

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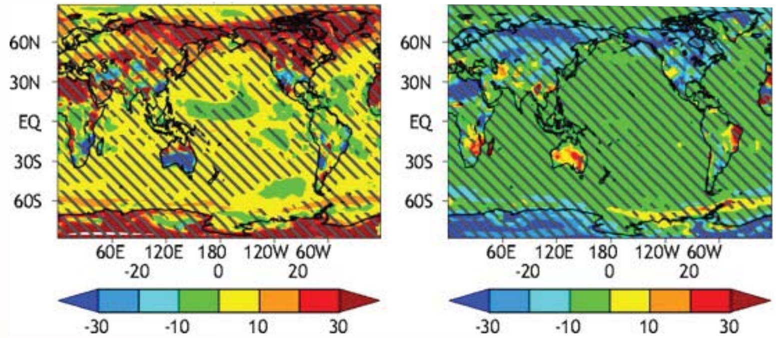
Adverse impact of geo-engineering schemes to mitigate climate change

PLS researchers have investigated the potential impact of "geo-engineering" schemes that would mitigate climate change, caused by rapidly rising CO_2 levels in the atmosphere, by intentionally reducing solar radiation incident on Earth's surface. Using equilibrium climate simulations, they showed that insolation reductions sufficient to offset global-scale temperature increases lead to a decrease in global mean precipitation. This occurs because solar forcing is more effective in driving changes in global mean evaporation than is CO_2 forcing of a similar magnitude. For the climate model used in their simulations, the researchers found that the change in global mean precipitation per degree warming is 2.4% per degree for solar forcing, but only 1.5% per degree for CO_2 forcing. Although other models and the climate system itself may differ quantitatively from this result, the qualitative conclusion is supported by simple considerations of the energy budget at Earth's surface. For a given change in surface temperature, changes in insolation result in relatively larger changes in net radiative fluxes at the surface; these are compensated for by larger changes in the sum of latent and sensible heat fluxes. Hence, the hydrological cycle is more sensitive to temperature adjustment due to changes in insolation than due to changes in greenhouse gases. This implies that geo-engineering schemes designed to alter solar forcing might offset temperature changes or hydrological changes from greenhouse warming, but could not cancel both at once. This research appeared in the June 3, 2008 edition of the ***Proceedings of the National Academy of Sciences.***

Besides a reduction in the rate of global mean water cycling, there are other reasons to be cautious about geo-engineering schemes for climate stabilization. For example, such a scheme would not mitigate the harmful effects of ocean acidification if it does not reduce concentration of atmospheric CO_2. Some schemes could adversely impact the ozone layer. Because CO_2-induced climate change occurs over centuries, a geo-engineering scheme, if implemented, would have to be maintained over a very long time.



Changes in annual-mean surface latent heat flux (in percent) for the case of doubled CO_2 concentration (left) and the geoengineering stabilized case (right). Hatching indicates the regions where the changes are significant at the 1% level. Surface latent heat flux changes are significant over 61% the globe for doubled CO_2. There is a general decrease in latent heat flux over most of the regions in the stabilized case, suggesting that geoengineering will lead to a weakened hydrological cycle

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Improved model of multidecadal ocean warming and sea-level rise

An international team, including researchers from Livermore, the Centre for Australian Weather and Climate Research, and the Antarctic Climate and Ecosystems Cooperative Research Centre, captured and analyzed data from multiple independent observations of ocean temperatures and from 13 different modeling groups to estimate ocean heat content and associated sea-level changes from 1950 to 2003. They used statistical techniques that allow for sparse data coverage and applied recently developed corrections to reduce systematic biases in the most common ocean temperature observations. Their analysis—published in the June 19, 2008 edition of ***Nature***—suggests that ocean temperature and associated thermal expansion for the period 1961–2003 were 50 percent greater than had been estimated in the most recent International Panel on Climate Change report. With these new estimates, the decadal variability of the climate models with volcanic forcing now agrees approximately, on average, with the observations, but the multidecadal trends predicted by the models are still smaller than observed. These results suggest a continuing need for careful quality control of observational data, and also for detailed comparisons of observational estimates with climate models on global and regional scales, to understand the implications for the detection, attribution and projection of the rise in sea-level and climate change.

PLS contributions to this research involved the analysis of the different climate models, drawing upon archived data from the Climate Model Diagnosis and Intercomparison Program sponsored by the Department of Energy (DOE).

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New method distinguishes different kinds of seismic events

Using data from the collapse of the Crandall Canyon Mine in Utah that occurred on August 6, 2007, researchers from Lawrence Livermore and the University of California's Berkeley Seismological Laboratory have successfully applied a full waveform-matching technique to determine the source of seismic events. The team's results, which were published in the July 11, 2008 issue of ***Science***, indicate that seismic signatures can distinguish disturbances caused by nuclear explosions, earthquakes, and collapse events.

The tragic collapse of the coal mine in Utah killed six miners and three rescue workers. The 3.9-magnitude event was recorded at seismic stations operated by the U.S. Geological Survey and the National Science Foundation's Earthscope USArray. At the time, the research team was already developing a full waveform-matching technique to distinguish events by their seismic signals and decided to apply the technique to the Crandall Canyon data.

When the researchers compared the field observations to the modeling results, the Crandall Canyon seismograms clearly matched those calculated for a collapse event. The team also detected Love waves, surface seismic waves that cause horizontal shifting of the earth. Love waves are typically small in large mine collapses, but those from the Crandall Canyon collapse were larger than expected for a purely vertical collapse caused by gravity. One explanation, consistent with the data, is that the collapse was uneven, with one side closing more than the other. The seismic signals from the mine collapse were relatively small in magnitude. The fact that the researchers could identify the source the Crandall Canyon event from its seismic signature gives them confidence that they can use the waveform-matching technique to identify even relatively small underground nuclear explosions as part of nonproliferation efforts.

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Analysis of temperature trends in the tropical troposphere

A large collaboration of atmospheric scientists, including researchers from Livermore, have completed a new analysis of the previously identified and controversial discrepancy between modeled and observed trends in tropical lapse rates. Early versions of satellite and radiosonde temperature datasets suggested that the tropical surface had warmed more than the troposphere, while climate models consistently showed tropospheric amplification of surface warming in response to human-caused increases in greenhouse gases. A 2006 report of the U.S. Climate Change Science Program identified this as a "potentially serious inconsistency."

Using new observational estimates of surface and tropospheric temperature changes, the team found that there is no longer a serious discrepancy, within statistical uncertainty, between modeled and observed trends in tropical lapse rates. This emerging reconciliation of models and observations has two primary explanations. First, because of changes in the treatment of buoy and satellite information, new surface temperature datasets yield slightly reduced tropical warming relative to earlier versions. Second, recently developed satellite and radiosonde datasets show larger warming of the tropical lower troposphere. In the case of a new satellite dataset generated by Remote Sensing Systems (RSS) in Santa Rosa, California, enhanced warming of the troposhere is due to an improved procedure of adjusting the raw satellite data for inter-satellite biases. When the tropospheric temperature trend derived from RSS is compared with four different observation-based estimates of the changes in surface temperature, the surface warming is invariably amplified in the tropical troposphere, consistent with results from the climate simulations. While significant progress has been made to better understand the multi-decadal trends in tropical lapse rates, the large structural uncertainties in observations make it nearly impossible to completely reconcile the divergent observational estimates of temperature changes in the tropical troposphere. This research appeared in the November 15, 2008 edition of the ***International Journal of Climatology***.

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Characterizing the shallow subsurface in the Las Vegas Valley

A team of researchers from Lawrence Livermore, the University of Nevada Las Vegas, and three engineering organizations has developed a first-generation three-dimensional shear-velocity map for the Las Vegas Valley in Nevada. Shallow shear-wave velocity structure profoundly influences ground motion caused by earthquakes and is essential for site-specific analysis of the associated hazards. Using surface-based seismic methods to build shear-wave velocity profiles for the Las Vegas area is challenging because the shallow subsurface is quite heterogeneous and the depth to the underlying bedrock remains poorly constrained.

The researchers combined two complementary seismic methods—spectral analysis and multi-channel analysis of surface waves—to determine the wave velocities at twelve sites across the valley. An instrumented sledgehammer was used to generate the waves for measurements of the velocity profiles to a depth of 10 meters and to lateral distances of up to 8 meters. A 2040-kilogram dropped weight was the active source for measurements to a depth of 30 meters and to lateral distances of up to 80 meters. The multichannel analysis allowed for incorporation of passive source data. To extend coverage across the valley, the team augmented their datasets for the twelve sites with 160 additional velocity profiles obtained during previous seismic classification of sites for land development.

The initial regional velocity map shows that in low-lying areas, where fine-grained sediments predominate in the shallow subsurface, shear-wave velocities of 300 meters per second (m/s) or less occur at the surface. Velocities remain below 700 m/s even at the Miocene–Oligocene boundary, hundreds of meters below. On the valley margins, recent alluvial deposits have higher velocities both on the surface and at depth. The velocity map shows realistic offsets associated with the faults that cut through the valley.

This research, which was highlighted on the cover of the November 2008 issue of ***The Leading Edge***, published by the ***Society of Exploration Geophysicists***, will help in better understanding ground motion hazards in a rapidly developing major city that faces a significant earthquake risk.

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Life Sciences

Rapid diagnosis of foot-and-mouth disease

In collaboration with the University of California at Davis, PLS researchers have developed a rapid test to diagnose foot-and-mouth disease and to distinguish it from clinically similar animal diseases. The prototype instrument uses amplification through multiplexed reverse-transcription polymerase chain reaction coupled with flow-cytometric detection to screen simultaneously for genetic material from seven disease-causing RNA and DNA viruses.

Researchers at the Institute for Animal Health's Pirbright Laboratory in the United Kingdom tested the prototype using 287 samples, including 248 samples from animals suspected of having foot-and-mouth disease collected from 65 countries between 1965 and 2006, and 39 true negative samples collected from healthy animals. Assays used in the diagnostic included several previously defined viral signatures as well as new signatures identified by KPATH, Livermore's bioinformatics software system. In initial tests, the multiplex assay had a diagnostic sensitivity to foot-and-mouth disease of 93.9 percent, which is close to the 98.1 percent achieved when two singlepex assays were combined. In addition, the PLS assay could reliably differentiate between the foot-and-mouth disease virus and other vesicular viruses, such as swine vesicular disease virus and vesicular exanthema of swine virus. Research is under way to optimize the prototype instrument's performance and to perform extensive validation on a variety of samples before licensing the technology for routine deployment. Because the technique tests for multiple viruses in one reaction, the new diagnostic will not only reduce the use of reagents and other resources but also increase confidence in the results. Aspects of this research were published in the March 2008 issue of the ***Journal of Clinical Microbiology*** and the October 2008 edition of the ***Journal of Virological Methods***.

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Effects of thyroid hormones on human breast cancer cell proliferation

The involvement of estrogens in breast cancer development and growth has been well established. However, the effects of thyroid hormones and their combined effects with estrogens are not well understood, although epidemiologic studies have revealed a possible association between thyroid dysfunction and breast cancer. Livermore researchers have investigated the response of human breast cancer cells to the thyroid hormone triiodothyronine—particularly its role in mediating cell proliferation and gene expression—and found that it may play a role in breast cancer development and progression. They demonstrated that triiodothyronine promoted cell proliferation in a dose-dependent manner in two specific cell lines and also enhanced cell proliferation induced by the estrogen 17 beta-estradiol. Co-administration of the estrogen receptor antagonist ICI suppressed both estradiol- and triiodothyronine-induced cell proliferation. Using an estrogen response element (ERE-) -mediated luciferase assay, the team determined that triiodothyronine was able to induce the activation of ERE-mediated gene expression in human breast adenocarcinoma cells, although to a much lesser degree than that induced by estradiol. Although in vitro and in vivo conditions differ substantially with regard to metabolism, receptor concentrations, and other variables, these results suggest that thyroid hormones play an important role in regulating the proliferation and gene expression of breast cancer cells and that there is interaction between the estradiol and triiodothyronine signaling systems. Significantly, the results also suggest that triiodothyronine may have the ability to mimic or enhance the effects of estrogen on breast cancer proliferation. This research appeared in the March 2008 edition of the ***Journal of Steroid Biochemistry & Molecular Biology***.

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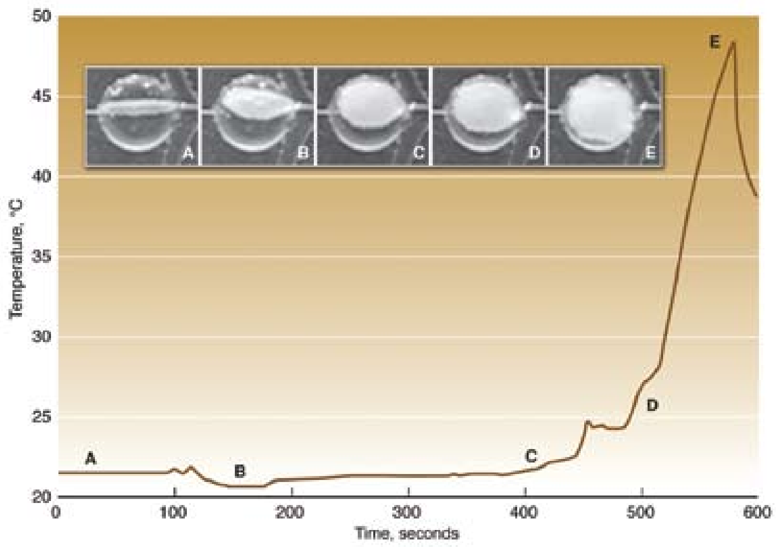
Developing a promising new treatment for aneurysms

Researchers in PLS are collaborating with colleagues from the University of California at Davis's Center for Biophotonics Science and Technology and from UC Berkeley to develop safer, faster, and more cost-effective treatments for patients with cerebral aneurysms, which are a major cause of strokes. The ideas is to isolate the aneurysm from the rest of the vascular system with one implanted device—a "plug" made from shape memory polymer (SMP) foam. SMPs are a class of polymeric materials that "remember" their original shape even after being molded into a temporary shape. Depending on its type, the SMP can then be restored to its original shape using heat, moisture, pH, or electric or magnetic fields; the Livermore-developed device is controlled with heat.

Researchers first cut a plug out of the foam material to match the contours of an aneurysm. They then use a crimping machine with heated blades to compress the foam plug into a stable temporary shape for delivery via a fiber-optic cable to the aneurysm sac. Once the plug reaches the sac, it is heated with diode-laser light through the fiber-optic cable. As the plug expands, it absorbs blood, which congeals and forms clots to stop blood flow inside the aneurysm.

Using an in vitro aneurysm model, the team has demonstrated that the technology is efficient in filling the aneurysm sac. A key feature of Livermore's SMP foam is its open-cell structure, which makes the foam very porous and absorbent. This allows fabrication of a foam plug that expands 80 to 90 times its compressed secondary shape. If the foam plug procedure is approved for clinical trials, researchers will be able to directly compare its efficacy with that of platinum coils—the currently most used technique. It could ultimately lead to a new, nonsurgical treatment option for patients. The foam plugs offer several potential advantages over platinum coils, including faster and more complete occlusion of the aneurysm and lower and more uniform stresses to the aneurysm wall, thereby decreasing the risk of hemorrhage.

Aspects of this research appeared in the March/April 2008 edition of the ***Journal of Biomedical Optics.*** In 2008, the research team received a 5-year grant from the National Institutes of Health to test the SMP devices on animals at Texas A&M University.



This graph shows the expansion of an SMP foam plug from its compressed secondary shape to its original shape in response to temperature changes over a period of about 10 minutes (A to E).

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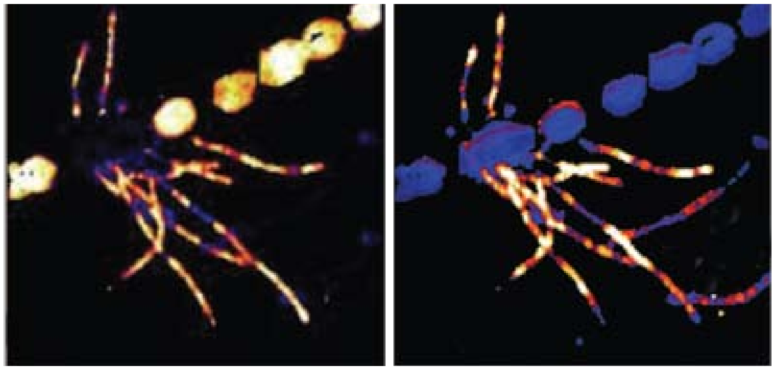
New method for probing individual cells in microbial communities

A team of researchers from Stanford University, Lawrence Livermore, the University of Oklahoma, and the Veterans Administration Hospital in Palo

Alto, California, has developed a new method for characterizing the phylogenetic identity and metabolic activity of individual cells in complex microbial communities. The method combines ribosomal RNA- (rRNA-) based in situ hybridization with stable atomic isotope imaging based on nanometer-scale secondary ion mass spectrometry (NanoSIMS). The researchers introduced fluorine or bromine atoms into cells using rRNA-targeted probes, which enabled phylogenetic identification of individual cells by NanoSIMS imaging. To overcome the natural fluorine and bromine backgrounds, they modified the in situ hybridization technique by using halogen-containing substrates, which enhanced the elemental labeling of microbial cells. The resulting relative cellular abundance of fluorine or bromine exceeded natural background concentrations by up to 180-fold, which improved the sensitivity of the isotopic imaging technique.



Images of a microbial consortium consisting of filamentous cyanobacteria and alphaproteobacteria attached to heterocysts obtained with nano secondary ion mass spectrometry (NanoSIMS). Color bars indicate distribution of ^{13}C as atom percent enrichment (left) and localization of fluorine relative to carbon (right).

To evaluate the new method, the team investigated interrelationships in a dual-species colonies consisting of a filamentous cyanobacterium and a heterotrophic alphaproteobacterium. The researchers also examined complex microbial aggregates obtained from human oral samples, in which they found evidence for metabolic interactions by visualizing the fate of substrates labeled with carbon-13 and nitrogen-15. This research—published in the May 2008 issue of ***Applied and Environmental Microbiology***—will help to understand the ecophysiology of known and uncultured microorganisms in complex environments and communities.

In addition, a quartet of visually striking scientific images resulting from this work will appear on the cover of all twelve 2009 issues of the ***International Society for Microbial Ecology Journal***. The images, which show a subregion of a cyanobacterial filament with attached parasitic bacteria, were selected from 40 nominations by a vote of the attendees at the 12th International Symposium on Microbial Ecology, held in August 2008 in Cairns, Australia.

Contact: Jennifer Pett-Ridge (925) 424-2882 (pettridge2@llnl.gov).

Understanding the interaction of insecticides with GABA receptor

Gamma-aminobutyric acid (GABA) is the chief inhibitory neurotransmitter in the central nervous system. Results from several experimental studies have shown that a series of chemically distinct insecticide compounds—such as picrotoxin, fipronil, and lindane—affect the $GABA_A$ receptor function. Using molecular dynamic simulation, PLS researchers have investigated the docking of this set of insecticides to the GABA receptor and identified five potential binding sites. The results of the simulations show that the lowest energy site is within the base of the transmembrane bundle, interacting with the M2 segment but not in the pore, and can accommodate many of the residues previously implicated in experimental studies of insecticide binding. Many of the binding modes are suggestive of a noncompetitive allosteric mechanism judging from interruption of the neurotransmitter channel gating mechanism, rather than directly blocking the channel. The results also distinguished between isomers of hexachlorohexane (HCH), finding that gamma-HCH (lindane) binds more favorably than beta-HCH. The simulations suggest multiple sites for insecticide binding and indicate the need for further mutagenesis and labeling work to either confirm or rule out the computational results. This research appeared in the May 2008 edition of the ***International Journal of Neuroscience.***

Contact: Felice Lightstone (925) 423-8657 (lightstone1@llnl.gov).

Understanding fat cell turnover in humans

The Center for Accelerator Mass Spectrometry in PLS has contributed significantly to a large international collaboration that investigated the factors determining fat mass in adult humans. In an article published in the June 5, 2008 edition of ***Nature***, the team reported the discovery that an adult human turns over approximately 10 percent of fat cells annually. The team also showed that the number of fat cells is a major determinant for the fat mass in adults. However, the number of fat cells stays constant in adulthood in lean and obese individuals, even after marked weight loss, indicating that the number of fat cells is set during childhood and adolescence. To establish the dynamics within the stable population of fat cells in adults, the researchers measured cell turnover by analyzing the incorporation of carbon-14—an isotope generated by atmospheric nuclear weapons tests—in genomic DNA. The results show that approximately 10 percent of fat cells are renewed annually at all adult ages and levels of body mass index. Neither cell death nor generation rate is altered in early onset obesity, suggesting a tight regulation of fat cell number in this condition during adulthood. The researchers concluded that the discovery of significant cell turnover, with regulated overall cell number, may lead to a new approach for therapeutic intervention in obesity.

This research was performed as part of a collaboration, underway since 2003, between the Center for Accelerator Mass Spectrometry at Livermore and the Karolinska Institute in Stockholm. Using the exceptional capability of accelerator mass spectrometry to measure very low concentrations of isotopes in very small samples, the collaboration had previously developed an innovative method to determine cell turnover in humans, based on the incorporation of carbon-14 isotope into genomic DNA. Levels of carbon-14 in the atmosphere were relatively stable until the Cold War, when above-ground nuclear weapons tests (1955–1963) caused a notable increase across the globe. Since 1963, carbon-14 levels have dropped exponentially due to diffusion from the atmosphere. Atmospheric carbon-14 is incorporated into plants by photosynthesis. By eating plants, and animals that live off plants, the carbon-14 concentration in the human body closely parallels that in the atmosphere at any given point in time. Because DNA is stable after a cell has gone through its last cell division, the carbon-14 level in DNA serves as a date mark for when a cell was born; this can be used retrospectively to determine the birth date of cells in humans.

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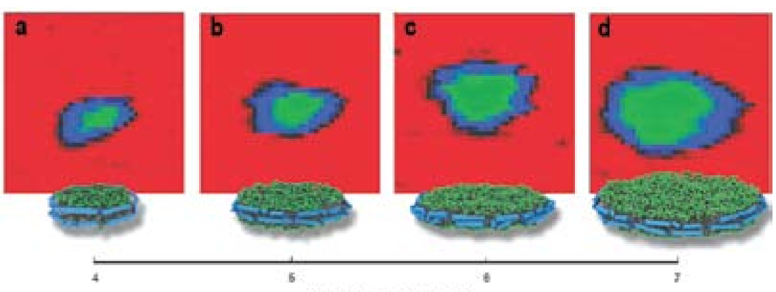
Characterizing the structure of nanolipoproteins

Combining their expertise in experimental and computational science, PLS researchers have characterized, at the nanometer scale, the structure of nanolipoproteins (NLPs), which are used as surrogates for cell membranes in studies of their interactions with viral and bacterial pathogens. The results of this research appeared in the July 2008 edition of the ***Journal of Lipid Research***. The experimental team used high-resolution techniques, such as atomic force microscopy, ion mobility spectroscopy, and electron microscopy, to image the thousands of NLPs they had assembled in the laboratory. In analyzing data from the experiments, they found that stable NLPs exist in four sizes. The different imaging methods gave remarkably similar results about NLP structure, which provided a starting point for the simulations.

As part of Livermore's Computing Grand Challenge Program, the computational team developed calculations to run on the Thunder and Zeus supercomputers. Using the experimental data, they first modeled the structure of an apolipoprotein called E4-22K, then simulated the dynamics of E4-22K apolipoproteins wrapping around a group of lipids to form the NLPs. The high-resolution models corroborated the experimental results that E4-22K NLP structures occur in four distinct sizes. This was the first time that scientists simulated biomolecular nanoparticles in so much detail. The computational results are also helping to determine the structure and function of membrane proteins.

In another paper, published in the November 2008 issue of ***Molecular & Cellular Proteomics***, the team described the novel technique used to prepare the membrane protein–containing NLPs in the laboratory. The technique relies on the rapid production of solubilized and functional membrane protein by simultaneous cell-free expression of an apolipoprotein and a membrane protein in the presence of lipids, leading to the self-assembly of NLPs. It has definite advantage over previous approaches, which require extensive efforts to express, purify, and solubilize the membrane protein prior to insertion into NLPs. In addition, a survey of membrane proteins co-expressed with a specific scaffold protein showed significantly increased solubility of all of the membrane proteins, indicating that this approach may provide a general method for expressing membrane proteins required for a variety of research efforts.

The NLP research program will advance scientists' understanding of how drugs interact with membrane protein receptors and the cells they affect—knowledge that is critical for developing potential treatments for diseases. In addition, it will help researchers evaluate cellular response to chemical and biological warfare agents, which will provide information required for developing improved countermeasures and approaches for detecting and minimizing the threat of exposure to these agents.



Atomic force microscopy images show that the number of protein chains surrounding a lipid determines the size of a nanolipoprotein (NLP). Research indicates that NLPs occur in four sizes: (a) 14.5, (b) 19.0, (c) 23.5, and (d) 28.0 nanometers in diameter.

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Observing the motion of a sliding biomolecule along DNA

PLS researchers and their collaborators at the Rockefeller University and Howard Hughes Medical Institute in New York have observed the motion of a polymerase III beta subunit—called a sliding clamp—loaded onto freely diffusing, single-stranded circular DNA annealed with fluorescently labeled DNA oligomers of up to 90 bases. DNA sliding clamps attach to polymerases and slide along DNA to allow rapid, processive replication of DNA. These clamps contain many positively charged fragments that could hinder the sliding because of attractive electrostatic interactions with the negatively charged DNA. The researchers measured the position and diffusion of the fluorescently labeled clamp on DNA using single-molecule fluorescence resonance energy transfer combined with alternating laser excitation. These techniques allow the team to observe the dynamic, unsynchronized movement of the sliding clamp on DNA.

Previous single-molecule measurements of other proteins sliding on DNA have tracked the position of the proteins on long DNA molecules that were tethered to a surface. The new measurements are an improvement over earlier experiments in two important aspects. First, the DNA is free-floating, not tethered to any surface, thereby avoiding any possible interference from interactions with the surface. Second, the experimental technique allows monitoring the short-range (1-to 10-nanometer) movements of the protein on DNA. The researchers found that the diffusion constant for the clamp moving along DNA is at least three orders of magnitude smaller than that for diffusion through water alone. They also found evidence that the fluorescently labeled beta clamp remains at the three prime end of the DNA in the presence of *Escherichia coli* single-stranded binding protein, suggesting that the clamp not only acts to hold the polymerase on the DNA but also prevents excessive drifting along the DNA. This research appeared in the August 22, 2008 issue of the ***Journal of Biological Chemistry.***

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People in the News

Valuing scientific excellence, leadership, and visibility

People in the News

The **Combustion Institute** honored **Charlie Westbrook** with its prestigious **Bernard Lewis Gold Medal**. The medal was inscribed with the words: "For brilliant research in the field of combustion, particularly on the pioneering development of detailed chemical kinetic mechanisms for use in practical applications." The award is named for Bernard Lewis, the head of the explosives branch of the U.S. Bureau of Mines in Pittsburgh, who founded the Combustion Institute in 1954. Westbrook, a retired PLS employee, has carried out chemical kinetic modeling studies since 1975, primarily in combustion of hydrocarbon fuels in many types of environments, with special focus on internal combustion engines.

Ken Moody, of the Chemical Sciences Division, was awarded the 2009 **Glenn T. Seaborg Award** by the **American Chemical Society**'s Division of Nuclear Chemistry and Technology for his work in heavy elements and nuclear forensics. He received his award at the organization's spring 2009 national meeting in Salt Lake City. Ken joined the Laboratory in 1985 and worked n the underground nuclear testing program until the test ban in 1992. After the test ban, he tapped into nuclear forensic analysis. At the same time, he was pursuing new super-heavy elements. With collaborators in Dubna, Russia, he helped discover elements 113–118.

Claire Max, a PLS alumna who helped pioneer adaptive optics (AO), has been **elected to the National Academy of Sciences**. Claire was the founding director of the Lab's Institute for Geophysics and Planetary Physics prior to leaving the Laboratory to serve as director of the Center for Adaptive Optics at UC Santa Cruz. She was one of 13 UC researchers elected to the academy in recognition of their distinguished and continuing achievements in original research. While at the Laboratory, Claire earned an E. O. Lawrence Award and was named an American Academy of Arts and Science fellow. Claire has made important contributions to the fields of plasma physics and astrophysics, and she is considered a central figure in the field of AO for ground-based telescopes.

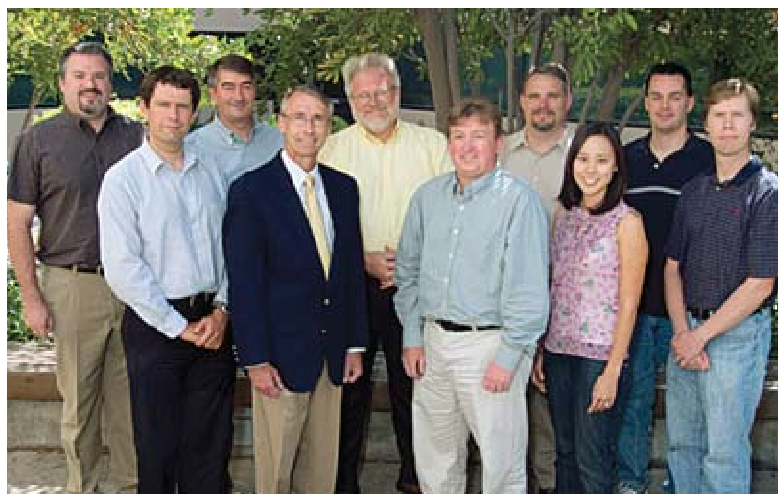
Don Correll was awarded the distinction of **fellow of the American Association for the Advancement of Science** (AAAS). Don is honored for his "longstanding recognition and distinguished contributions to science education, including communications and materials targeted toward students, teachers, and the general public." Correll is the director for the Institute for Laser Science Applications (ILSA) as part of the Associate Director's Office of the PLS Directorate. Don is also a fellow of the American Physical Society.

Per Söderlind was named a **fellow of the American Physical Society.** Per, of the Condensed Matter and Materials Division, has been at the Lab since 1994. He was honored for "important contributions in electronic-structure theory for transition and actinide metals, particularly plutonium." His first scientific publication, on plutonium and the light actinides, appeared in the APS journal *Physical Review B* in 1990. Earlier this year, Per received an LLNL award for his classified work on plutonium.

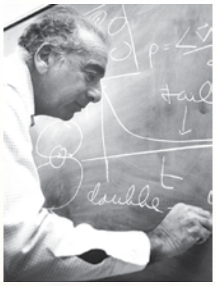
Bruce Goodwin (far left), principal associate director for Weapons and Complex Integration, stands with award winners from the Dual Axis Radiographic Hydrodynamic Test (DARHT) Support Team.

In the **DOE/NNSA Weapons Awards of Excellence, Ken Moody** (Chemical Sciences Division) won an **Individual Award** for Technical Excellence in Radiochemistry and Heavy Element Synthesis. Ken is an internationally recognized expert in radiochemistry and the synthesis of heavy elements. He is LLNL's most knowledgeable expert in developing and applying radiochemistry to stockpile stewardship activities and has made outstanding contributions toward improved understanding of weapons behavior. In addition, **George Caporaso, Frank Chambers, Yu-Jiuan Chen**, and **John Weir**, all from the Physics Division, were named in a **Team Award** (photo above) for Technical Excellence in Radiographic Hydrodynamics, for successfully designing, modeling, configuring and building the Dual Axis Radiographic Hydrodynamic Test (DARHT)-2 downstream electron-beam hardware and four-pulse targets for the DARHT second axis.

Researchers in PLS were part of one of three LLNL teams to win an **R&D 100 Award**, which are presented by *R&D Magazine* to the top 100 industrial innovations world wide in 2007. Often known as the "Oscars of invention," the 2008 R&D 100 awards were presented on October 16 during a black-tie dinner in the Grand Ballroom of Chicago's Navy Pier. **Wayne King, Nigel Browning, Geoffrey Campbell, Thomas LaGrange**, and **Bryan Reed**, of the Condensed Matter and Materials Division; **Michael Armstrong**, of the Chemical Sciences Division; and former Lawrence scholar **Judy Kim** were part of the team that developed the dynamic transmission electron microscope (DTEM), which provides the highest resolution ever for imaging of ultrafast material processes on the billionth-of-a-meter scale.



DTEM development team (from left): Thomas LaGrange, Bryan Reed, Geoffrey Campbell, Wayne King, William DeHope, Nigel Browning, Richard Shuttlesworth, Judy Kim, Benjamin Pyke, and Michael Armstrong. Not pictured: Brent Stuart, Mitra Taheri, J. Bradley Pesavento, and Benjamin Torralva.



Retired PLS physicist and computational pioneer **Berni Alder** was inducted as a **fellow of the American Academy of Arts and Sciences** at a ceremony in Boston, Massachusetts, on October 11, 2008. Alder is widely regarded as the founder of molecular dynamics, a type of computer simulation used for studying the motions and interactions of atoms over time. Among numerous other honors, he is a member of the National Academy of Sciences.

Multiple PLS researchers received a **2008 Nanotech 50 Award**. Presented by *Nanotech Briefs*—the monthly digital newsletter from Tech Briefs Media Group—the Nanotech 50 recognizes the top 50 technologies, products, and innovators that have significantly impacted, or are expected to impact, the state of the art in nanotechnology. The winners of the Nano 50 awards are the “best of the best”—the innovative people and designs that will move nanotechnology to key mainstream markets. **Alex Gash**, of the Chemical Sciences Division, was an awardee in the technology division for work involving the application of inorganic synthetic techniques to the formulation of energetic nanocomposites. **Yinmin Wang** won in the innovator category for his nanoscale research. Yinmin, who works in the Condensed Matter and Materials Division, focuses on the mechanical behavior of bulk nanostructured materials and nanolaminates, semi-conducting nanowires, the mass transport behavior of nanotubes, and transmission electron microscopy. **Paul Hoeprich** and **Matthew Coleman**, of the Biosciences and Biotechnology Division, were recognized for devising a technique for creating nanolipoprotein particles (NLPs), which consist of nanometer-sized complexes that enable the study of proteins that are particularly challenging to capture in the native form, due to being associated with cell membranes. Their NLPs have a protein ring around a lipid bilayer, which is similar to a cell membrane, and can reconstitute insoluble proteins. **Sonia Létant** was recognized for designing and fabricating functional nanopores. Working in the Chemical Sciences Division, Sonia developed a novel approach to fabricate artificial membranes with the goal of building a synthetic replicate of the protein channels used by living systems for molecular recognition followed by electrical transduction. **Nerine Cherepy** and **Joshua Kuntz**, of the Chemical Sciences Division, and **Jeff Roberts**, of Atmospheric, Earth and Energy Division, won for fabricating transparent ceramics from nanoparticles. The Nano 50 were presented at a special awards dinner held during the NASA Tech Briefs National Nano Engineering Conference in Boston on November 12–13.

Tony Makarewicz, of the Biosciences and Biotechnology Division, was one of three LLNL scientists to win an **Award for Excellence in Technology Transfer from the Federal Laboratory Consortium for Technology Transfer** in recognition for the Autonomous Pathogen Detection System (APDS). Completely autonomous, APDS uses both antibody and DNA methods, detects all bioagent types, and is capable of multiplex detection of potentially up to 100 channels.

Mark Sutton (Chemical Sciences Division), **Tom Wolery** (Atmospheric, Earth and Energy

Division), and **Sharon Torres** (Condensed Matter and Materials Division) received a **citation from DOE's Office of Civilian Radioactive Waste Management** (OCRWM) in recognition of their contributions to a major milestone in the Yucca Mountain Project. The award citation recognized their "contribution and support of the OCRWM Lead Laboratory for Repository Systems and the completion of a quality License Application and technical basis that is credible, defensible and respected, as delivered to the Department of Energy, April 2008" and was signed by the director of the OCRWM and other project officials.

George Miller (far left) with the S&T Award-winning computation team.

Fred Streitz and fellow computational scientists **Jim Glosli, Kyle Caspersen, David Richards**, and **Robert Rudd**—all of the Condensed Matter and Materials Division—were recognized by Laboratory Director George Miller with a 2008 **LLNL Science and Technology Award** for their "game changing" innovations. A continuous computer run of over one month was needed, according to Streitz—now the director of the Institute for Scientific Computing Research—who spoke on behalf of the S&T Award-winning teams at the October 10 ceremony. To conduct a simulation that long without the disruptions typical on a machine with as many processors as BlueGene/L—over 200,000 CPUs—required the development of a "fault-tolerant" application code that would eliminate delays in computer operation caused by the hardware failures that are inevitable on a massively parallel machine of that size and complexity. Using the application itself to correct hardware errors was the game-changing innovation that allowed the team to perform their extremely large-scale molecular dynamics simulations for very long times.

On October 10, a team of over 40 LLNL researchers who contributed to the Intergovernmental Panel on Climate Change (IPCC)—a co-winner of the 2007 Nobel Peace Prize—was presented by Director George Miller with a 2008 **LLNL Science and Technology Award**. The Laboratory's Program for Climate Model Diagnosis and Intercomparison (PCMDI) has made major contributions to all four Assessment Reports released by the IPCC between 1990 and 2007. The PLS team members awarded—all working in the Atmospheric, Earth and Energy Division—were PCMDI lead investigator **Dave Bader** and teammates **Celine J. W. Bonfils, James S. Boyle, Philip J. Cameron-Smith, Chien-Hua Chuang, Curtis C. Covey, Philip Duffy, Peter Gleckler, Stephen Klein, Thomas J. Phillips, Benjamin Santer, Kenneth R. Sperber**, and **Karl Taylor**.

The Lab climate team that contributed to the Scientific Assessment Reports of the intergovernmental Panel on Climate Change (IPCC) with Director George Miller (far right).

Karl van Bibber was elected vice chair of the American Physical Society's (APS's) California Section. As one of eight regional sections nationwide, the APS California section hosts multidisciplinary meetings in Northern and Southern California. The rotating location helps minimize travel expenses for scientists who wish to join colleagues. The 2008 section meeting drew 200 attendees to Berkeley, where the Laboratory's **Hope Ishii** spoke about her materials science approach to isolating comet dust from the Wild 2 mission for analysis. Karl became a fellow of the APS in 2007 and is also a fellow of the American Association for the Advancement of Science.

The team members who have developed and advanced the Autonomous Pathogen Detection System are, left to right: Dean Hadley, John Dzenitis, Shanavaz Nasarabadi, Vincent Riot, Elizabeth Wheeler, Tony Makarewicz, Chris Bailey, Todd Corzett and Todd Weisgraber. Not pictured are John Breneman, Sally Hall, Christine Hara, Bruce Henderer, Staci Kane, Tom Metz, Pejman Naraghi-Arani and Jason Olivas.

The LLNL team that developed and deployed the Autonomous Pathogen Detection System (APDS)—for detecting the terrorist usage of biological agents—was **honored by the Global Security principal directorate** on the one-year anniversary of the system's use in the Department of Homeland Security's BioWatch Program. For the past 12 months, APDS has been deployed in a major East Coast city. "The future is very bright," said John Doesburg, the principal associate director for Global Security. The APDS team is led by John Dzenitis, of the Engineering Directorate. Team members from PLS—who all work in the Biosciences and Biotechnology Division—are **Shanavaz Nasarabadi, Tony Makarewicz, Chris Bailey, Todd Corzett, Sally Hall, Christine Hara, Staci Kane, Pejman Naraghi-Arani**, and **Jason Olivas**.

Of the five Laboratory researchers **selected by the American Physical Society (APS) as outstanding referees of APS journals**, three were PLS scientists: **Peter Beiersdorfer, Mau Hsiung Chen**, and **Ian Thompson**, of the Physics Division. The APS "outstanding referee" program was instituted in 2008. The highly selective award program recognizes scientists who have been exceptionally helpful in assessing manuscripts for publication in APS journals. Beginning next year, the program will recognize approximately 130 of the 42,000 currently active referees annually, but in this inaugural year, a larger group of 534 referees was selected. Through this program, APS expresses its appreciation to all referees, whose efforts in peer review not only keep the standards of the journals at a high level, but in many cases also help authors to improve the quality and readability of their articles—even those that are not published by APS. The final 534 honorees were selected on the basis of the quality, number, and timeliness of their reports, without regard for membership in the APS, country of origin, or field of research. The APS also recognized the outstanding referees during the prize and award session at the 2008 APS March meeting in New Orleans and at the April meeting in St. Louis.

Lab researcher **Kevin Fournier** was part of a team that won the **2007 "Outstanding Paper" award at the Hardened Electronics and Radiation Technology (HEART) Conference** held in Colorado Springs. Fournier, a 14-year Lab employee in the Physics Division, co-authored the paper "Analysis of Cavity SGEMP [system generated electro magnetic pulse] Experiments at the Omega Laser Facility," with researchers from ITT Advanced Engineering & Sciences, Sandia National Laboratories, and Atomic Weapons Establishment in the U.K. The HEART annual conference is the largest gathering of DoD contractors and program people involved in radiation-hardening technology.

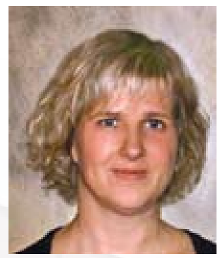
Joseph Morris and **Lewis Glenn**, of the Atmospheric, Earth and Energy Division (AEED), were part of a five-author team that won the 2007 **Award for Best Applied Research from the American Rock Mechanics Association** for the article "Simulations of Underground Structures Subjected to Dynamic Loading, Using the Distinct Element Method," which appeared in *Engineering Computations* in 2004. The other three authors were retired AEED scientists **Francois Heuze** and **Stephen Blair,** and **Miles Rubin**, a visiting faculty scholar in AEED (not shown). The award was announced in Vancouver on May 29, 2008, at the 1st Canada–U.S. rock mechanics symposium and was given to the authors at the U.S. Rock Mechanics Symposium held in San Francisco, June 29–July 2, 2008.

For her many achievements—including overseeing the Lab's agricultural assay development work and its foreign animal disease modeling program—**Pam Hullinger was inducted into the Alameda County Women's Hall of Fame.** One of seven women to be inducted in 2008, Hullinger, who works in the Biosciences and Biotechnology Division, was recognized for skills as a veterinarian and for her expertise in fighting the spread of animal infectious diseases on the front lines for two of the world's major outbreaks of animal disease—foot-and-mouth disease (FMD) in Great Britain in 2001 and exotic Newcastle disease in California in 2002 and 2003. Pam is an associate clinical professor in the UC Davis School of Veterinary Medicine and an adjunct member of the graduate faculty in Texas A&M's Veterinary Integrative Biosciences Department.

Russell Wallace received the 2008 Larry Foreman Award for “Innovation and Excellence in Target Fabrication” at the 18th Target Fabrication Meeting in Lake Tahoe. The award recognizes Wallace’s record of outstanding support to laser experiments using the Nova laser, the Omega laser, and NIF. The award is given out approximately every two years since 1999 in memory of Larry Foreman, formerly of Los Alamos National Laboratory, and his innovative work in target fabrication for inertial confinement fusion.

Larry Thompson (right) receives the Environmental Mutagen Society award from EMS President Andrew Wyrobek.

Larry Thompson, a molecular biologist in the Biosciences and Biotechnology Division, **received the 2008 Environmental Mutagen Society (EMS) Award**. The award is given to one individual annually by the EMS in recognition of “outstanding research contributions in the area of environmental mutagenesis.” The award was presented at the EMS annual meeting in Puerto Rico. Thompson was selected for the award from a pool of nominees, which included non-EMS members. His research during his more than 35 years at LLNL has focused on the biological processes by which DNA is repaired in vivo. Specifically cited by the EMS was his “application of mammalian somatic cell genetics to the study of mutagenesis and the cloning of DNA repair genes.”



Christine Orme, a staff scientist in the Biosciences and Biotechnology Division, **has been elected to the board of the Materials Research Society** (MRS), an organization of materials researchers from academia, industry, and government. The society promotes communication for the advancement of interdisciplinary materials research. Orme joined the MRS as a graduate student, giving one of her first invited talks at an MRS meeting. More recently, Orme has served as a conference co-chair, symposium organizer, and volume organizer, editing material for the monthly ***MRS Bulletin***.

Lisa Poyneer, of the Physics Division and the Engineering Directorate, **was awarded the Jain Prize from UC Davis** for her dissertation, “Signal Processing for High-Precision Wavefront Control in Adaptive Optics.” The annual award recognizes the best Ph.D. dissertation in the UC Davis Electrical and Computer Engineering Department. Innovations described in her dissertation include the spatially filtered wavefront sensor, which prevents aliasing, and a predictive wavefront controller, which uses Kalman filtering to keep up with the turbulent atmosphere. Her research helped the Laboratory secure a $24 million contract to build the Gemini Planet Imager.

Judy Kim, a graduate student at UC Davis majoring in materials science and engineering and a former Lawrence scholar in the Materials Science and Technology Division, **received the John Farrant Memorial Award** for her abstract and research entitled "Nanosecond Imaging in the Dynamic TEM Reveals Unquenchable Transient Microstructure." The award is presented to a student who has demonstrated a scientifically significant study in the physical sciences. This was Kim's third year at LLNL working in the area of transmission electron microscopy.

Kennedy Reed (Physics Division) was invited to participate in the **Workshop on Science, Technology and Innovation held in connection with Sullivan Summit VIII** in Arusha, Tanzania. The Leon H. Sullivan Summits bring together the world's political and business leaders, delegates representing national and international civil and multinational organizations, and members of academic institutions to promote partnerships between African and American scientists in areas of basic sciences, technology, and engineering. Kennedy was also one of six U.S. physicists **appointed by the National Academy of Sciences (NAS) to serve as a U.S. delegate to the General Assembly of the International Union of Pure and Applied Physics** (IUPAP), held October 14–18 in Tsukuba, Japan. At the General Assembly, Reed was elected Chair of the IUPAP Commission on Physics for Development, which works to promote physics and physicists in developing regions of the world, and to facilitate the exchange of relevant information throughout the international scientific community.

From left, front: Dan White, Michael Thelen, Malvin Kalos and Eivind Almaas. (From left, back):Lab Deputy Director Steve Liedle, Patrick Brantley, Dustin Froula, Ming Jiang, Richard Johnson, and Wren Carr.

Four of the 11 Lab recipients of the **Department of Energy's (DOE) Outstanding Mentor Award** were PLS researchers—**Pam Hullinger** (Biosciences and Biotechnology Division); **Eivind Almaas** and **Michael Thelen** (Biosciences and Biotechnology Division); and **Ted Laurence** (Condensed Matter and Materials Division). The DOE Outstanding Mentor Award began in 2002 as an effort to establish a culture that values mentorship within the DOE national laboratories. This year a total of 83 awards were presented to recipients from DOE national laboratories. Mentors dedicate time and attention to providing well-defined research projects for summer students that match the student's research interests and supportive materials. What makes the awards unique is that the recipients are nominated by the summer students they mentored. Nominations are solicited from students near the end of the summer. DOE provides five core criteria to evaluate nominations, and LLNL has supplemented these with an additional five.

Daniel Decman, of the Chemical Sciences Division, **was appointed to DOE's Isotopes Subcommittee**, a newly formed standing subcommittee of the Nuclear Science Advisory Committee. The subcommittee will advise the DOE about the potential transfer of the DOE Isotope Production Program from DOE's Office of Nuclear Energy to the Office of Science. Chaired by Donald Geesaman of Argonne National Lab and Professor Ani Aprahamian of Notre Dame, the subcommittee will produce two reports that will identify research opportunities involving isotopes and provide a 10-year strategic plan.

The Physics Division's **Steve Allen was elected to the office of 2009 Vice Chair of the American Physical Society Division of Plasma Physics** (DPP). The 2009 DPP Vice Chair automatically becomes the 2010 Chair-Elect and then the 2011 Chair of the DPP. DPP is one of 14 APS divisions that provide opportunities for members to interact with colleagues with similar interests and to keep abreast of new developments in their specialized fields. The annual meeting of the DPP is one of the key meetings each year attended by the research staff at LLNL.

Tom Casper, of the Physics Division, **was selected for a senior position at the International Thermonuclear Experimental Reactor (ITER) Center** in Cadarache, France. His title there will be Scientific Officer, Equilibrium and Control, Fusion Science and Technology. Casper will report to the ITER Assistant Deputy Director General and Deputy Director General for Fusion Science and Technology and will be responsible for analysis of ITER requirements and performance in the areas of plasma equilibrium, evolution, and control. Casper has been with LLNL's Fusion Energy Program since 1978.

James Tobin, of the Condensed Matter and Materials Division, was recently **elected as one of four 2009 Executive Committee members of the Magnetic Interface and Nanostructure Division of the American Vacuum Society** (AVS). The AVS and its divisions comprise one of nine member societies of the American Institute of Physics.

The Physics Division's **Marilyn Schneider** was one of two national laboratory employees recently **elected to the executive committee of Omega Laser Users Group**. The committee—which defines all aspects of the OLUG bylaws, policies, and procedures—is comprised of four members from the academic and small business community, two from the national laboratories, one international member, one member (selected by the other committee members) with extensive experience in a user group at a major existing facility (e.g., a light source), and one ex officio member chosen by the Laboratory for Laser Energetics in Rochester, New York.

Announcements in the News

Strengthening science and technology for national needs

Announcements in the News

Assessment of climate models issued

The U.S. Climate Change Science Program, a federal interagency initiative, issued the tenth report in a series of 21 Synthesis and Assessment Products to be issued over several years. The report—*Climate Models: An Assessment of Strengths and Limitations*—is one of only two of the planned reports to focus on computational modeling. The report explored the strengths and weaknesses of the various computational models being used to simulate climate change. In addition to addressing the individual models, the report concluded that, in aggregate, the multiple models produced results of high quality when applied at continental or greater spatial scales. Dave Bader, of PLS, was the coordinating lead author of the report, along with seven other authors, including PLS researcher Curt Covey. The report represents an assessment by 29 experts spanning the field as part of the Federal Advisory Committee chartered by the Department of Energy (DOE). The release of the DOE report was announced at a July 31, 2008 teleconference with the press, with Dave Bader representing the computational climate science community. The second report addressing computational predictions of climate change will be published by the National Oceanic and Atmospheric Administration.

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Award opens door to promising partnership with biotech firm

On August 29, 2008, the National Institute of Allergy and Infectious Disease announced four major contracts resulting from a 2007 solicitation titled “Development of Therapeutic Agents for Select Biodefense Pathogens.” One is a 5-year, $27.6 million contract with San Diego-based Trius Therapeutics. Three PLS scientists—Felice Lightstone, Ken Turtletaub, and Paul Jackson—expect to assist Trius in the respective areas of computational biology, pharmacology using accelerator mass spectrometry, and select agents. Pending the approval of a funds-in cooperative research and development agreement, the Laboratory will receive a total of approximately $1 million annually for 4 years. The partnership with Trius resulted from discussions at an advisory group meeting regarding new ideas and future directions for biology research at Livermore.

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Axion Dark Matter Experiment upgrade completed and data-taking begun

The second-generation Axion Dark Matter Experiment (ADMX) at Livermore was commissioned and began a year-long data-taking experiment on March 28, 2008. ADMX is one of the leading experiments in the world searching for dark matter in the universe—and the only one currently looking for axions, a hypothetical elementary particle believed to be extremely light and possessing extraordinarily weak couplings to matter and radiation. ADMX, led by PLS scientists, is a collaboration of researchers from Livermore, MIT, University of Florida, Lawrence Berkeley National Laboratory, University of California at Berkeley, University of Chicago, and Fermilab. The team constructed the first-generation Livermore device to search for axions in the mid-1990s using a cylindrical radio-frequency cavity and heterostructure field-effect transistor amplifiers cooled to 1.3 kelvin. The subsequent experiments have set an improved upper limit for the axion coupling constant in a limited axion mass range. The DOE Office of High Energy Physics funded a 4-year, $2 million upgrade to the experiment, starting in July 2004, to rebuild the apparatus with an entirely new and revolutionary type of amplifier—a quantum-limited superconducting quantum interference device (SQUID). This technology provides for a significantly lower noise temperature in the device, allowing the scientists to search for axions with improved sensitivity. In a related project, the Intelligence Advanced Research Projects Agency has begun funding research in PLS to explore and develop SQUIDs for future applications in quantum information and computing.

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Carbon storage technology to be fielded

The Laboratory and American Shale Oil (AMSO), a subsidiary of IDT Corporation, entered into an agreement to develop carbon sequestration technologies for in-ground shale oil production processes. The Livermore team, led by PLS researchers, will study how to use depleted underground oil shale retorts—refractory chambers where oil shale is heated—to permanently store carbon dioxide. Oil shale can be converted to oil by subjecting it to high temperatures and pressures. The shale that remains in the ground after the oil is extracted could be used as a storage place for the carbon dioxide that is created during the extraction process. This project utilizes a Livermore-developed model of how oil is formed in nature—a model that aids the exploration efforts of every major oil company in the world. The partnership with AMSO is in line with the Laboratory's mission in energy and environmental security for the nation. The LLNL–AMSO technology will be demonstrated in northwest Colorado's oil shale–rich Piceance Basin, where AMSO has leased a 160-acre parcel of federal land from the U.S. Bureau of Land Management.

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Dark matter collaboration receives DOE and NSF funding

The Large Underground Xenon (LUX) Dark Matter Project, a collaboration of Lawrence Livermore, Brown University, Case Western Reserve University, University of California at Davis, Yale University, and others was approved for joint Department of Energy–National Science Foundation funding. The LUX project will be among the first experiments conducted at the Sanford Underground Science and Engineering Laboratory at the Homestake Mine in South Dakota, which will become the U.S. Deep Underground Science and Engineering Laboratory in 2012. LUX will use a dual-phase liquid xenon detector to search for weakly interacting massive particles (WIMPs) with unprecedented sensitivity. WIMPs are thought to be free of electric charge and thus nonluminous—i.e., dark—to have a mass in the range of 0.1–1 teraelectronvolts, to have very weak interactions with matter, and to permeate the universe. PLS members of the collaboration are designing and testing the analog front-end electronics for the large detector, building key elements of the detector interior and shield, and providing an extensive detector simulation framework that takes advantage of Livermore's uniquely powerful computing resources.

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Developing advanced point-of-care diagnostics

Lawrence Livermore and the UC Davis Health Center are collaborating to develop and test point-of-care diagnostic instruments for use in hospitals, rural areas, and disaster sites. Through a 5-year grant from the National Institute of Biomedical Imaging and Bioengineering, the team is working on two prototype instruments that simultaneously detect five bacterial and fungal pathogens: methicillin-resistant *Staphylococcus aureus, Pseudomonas aeruginosa, Escherichia coli, Streptococcus pneumoniae,* and *Candida* yeast. PLS researchers are developing unique DNA signatures or assays for use with the new instruments, which will process blood samples using a new method called loop-mediated amplification to simultaneously test for all five pathogens in an hour. Techniques and components demonstrated previously in other Livermore biodetection technologies, such as the Autonomous Pathogen Detection System, are helping to speed the development of the new instruments, which must be easy to use and require minimal user training for widespread deployment. To help prepare the nation for disasters, the Livermore–UC Davis team is also evaluating exploratory diagnostic technologies.

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First light from T-REX

Livermore's Thomson-Radiated Extreme X-ray Source (T-REX)—developed jointly by the National Ignition Facility and Photon Science Principle Directorate and PLS—produced an intense burst of gamma-rays for the first time on March 26, 2008, making it the brightest such instrument in the world in the 0.7–1.0 megaelectronvolt (MeV) energy range. T-REX uses scattered relativistic electrons to produce monochromatic, highly collimated, tunable x rays and gamma rays. To achieve "first light," the system's 120-MeV electron beam, in a 10-picosecond pulse, collided with ultraviolet laser photons to produce gamma-rays with energy of 0.776 MeV. Traditionally, beams in this energy regime are created in synchrotron facilities, but T-REX's peak brightness will be up to 10 orders of magnitude greater than current third-generation synchrotron light sources. T-REX will be able to identify specific nuclei and isotopes through a process called nuclear resonance fluorescence (NRF), allowing researchers to address challenges in homeland and international security, nonproliferation, advanced nuclear power systems, and nuclear waste identification. The Department of Homeland Security is funding research at Livermore to explore the possible use of an NRF-based system to detect nuclear materials in well-shielded objects. A system based on T-REX technology could provide a solution for detecting concealed highly enriched uranium in cargo containers.

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Forensic Science Center clears chemical weapons challenge

The Forensic Science Center participated informally in the 24th test sponsored by the Organization for the Prohibition of Chemical Weapons (OPCW), which involved identifying a reportable compound mixed into an interfering organic matrix (diesel fuel). The specific target compound was not listed in common mass spectral databases, making the identification of the compound especially challenging. Nevertheless, using the unique capabilities of the Forensic Science Center in PLS, the Livermore team completed the analysis and submitted its report to the OPCW on time. The Forensic Science Center is one of only two laboratories in the U.S. certified by the international community for identifying chemical-warfare agents.

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Gulf War syndrome report cites PLS research

A report entitled *Gulf War Illness and the Health of Gulf War Veterans: Scientific Findings and Recommendations*, which was released in November 2008 by the congressionally mandated Research Advisory Committee on Gulf War Veterans' Illnesses, made several references to research done at the Center for Accelerator Mass Spectrometry (CAMS) in PLS. The report cited an ongoing collaboration with the University of New Mexico studying the inhalation penetration of depleted uranium into brain tissues. It described toxicity studies at CAMS that supported the overall conclusion that a chemical given to the troops for protection against nerve agents and pesticide use during deployment are "causally associated with Gulf War illness." The report also cited two previous CAMS publications: "Pyrethroid decrease in central nervous system from nerve agent pretreatment" [***Journal of Applied Toxicology*** (1997)] and "Protein binding of isofluorophate in vivo after coexposure to multiple chemicals" [***Environmental Health Perspectives*** (2002)].

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LSST primary–tertiary mirror declared “perfect”

The Large Synoptic Survey Telescope (LSST) project, managed by Donald Sweeney from PLS, announced on July 24, 2008, that the primary–tertiary mirror casting appeared to be “perfect” when the furnace lid was removed on the previous day. The mirror had been cooling for 100 days since completing its successful “high fire” in March to allow the mirror to anneal and cool gradually to room temperature. The casting of the mirror was done at the Steward Observatory Mirror Laboratory at the University of Arizona. Lawrence Livermore is a major institutional partner in the LSST project, with official responsibility for several aspects of the LSST design and development that leverage unique LLNL capabilities in optical engineering and high-performance computing. PLS researchers also play a leadership role in planning the telescope’s scientific use. When operational, the LSST will address a wide range of pressing scientific questions, including: What is dark energy? What is dark matter? How did the Milky Way form? What are the properties of small bodies in the solar system? Are there potentially hazardous asteroids that may impact the earth causing significant damage?

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New nuclear data library released

A team of PLS scientists have completed and released a nuclear database that incorporates evaluated data from Livermore and from various nuclear physics programs around the world. The data library—the culmination of a multiyear project—sets a new standard for providing the nuclear data needed for weapons and nonproliferation. The library includes some 500 evaluations (roughly four times the number in the previous standard database) and many physics improvements important for calculating weapon performance, output effects, attribution signatures, radiochemical diagnostics, and the performance of conventional and hybrid fission–fusion reactors.

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Radiation technology hits the road

State and local government agencies have begun to deploy a radiation detector originally developed by Livermore scientists and engineers. The device, called the adaptable radiation area monitor (ARAM), is being used to monitor for nuclear materials that could be part of a “dirty bomb” or nuclear device. The ARAM system can detect concealed radioactive material about the size of a grain of sand moving at nearly freeway speed. The technology was licensed to—and converted into counterterrorism tools by—Textron Defense Systems Corporation, in Wilmington, Massachusetts. One state in the Western U.S. has deployed more than 20 ARAM systems at state vehicular entrances to monitor for nuclear materials. A second state, New Jersey, has acquired from Textron a fleet of ARAM-equipped sport utility vehicles to patrol its highways and streets looking for nuclear materials. Known as RadTrucks, the vehicles have been in operation since the state joined multiple agencies in the New York City region as part of a federal pilot program to detect terrorist nuclear material before it can be detonated. The Department of Homeland Security provides grants for such projects through its Securing the Cities Initiative to enhance regional capabilities for detecting and interdicting illicit radioactive materials.

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